BRL

REPORT NO. 1617

NUMERICAL MODEL FOR DRIFT TUBE ANALYSIS

by

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October 1972

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B A L L I S T I C R E S E A R C H L A B O R A T O R I E S

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Concepts Analysis Laboratory

RDT&E Project No. 1T061102B53A/15

A B E R D E E N P R O V I N G G R O U N D, M A R Y L A N D

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Aberdeen Proving Ground, Md
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ABSTRACT

A FORTRAN IV program has been written which uses an iterative technique to model ion transport and chemistry in a drift tube. The program, named MULTIGATE, uses finite difference calculus to generate time arrival histories at several points in the drift space for the case of three ion species undergoing populating and depopulating reactions and at the same time drifting with the electric field and diffusing in the radial and axial directions. To facilitate comparison with drift tube data, the computer output includes plots of the ionic currents versus time.

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GLOSSARY

Throughout the glossary the symbol A is used to refer to ion species A. The symbols B or C may be substituted to form the FORTRAN variable names applying to ion species B or C. Likewise, the symbol "k" may be replaced by the symbol "1," "2," "3," "4," or a blank to refer to the four intermediate and the final gates in the list of FORTRAN variable names.

A	calculated value of the density at time T of ion species A
AP	time derivative of the density at time T of ion species A
PA	predicted value of the density at time T+DT of ion species A
APP	time derivative of the predicted density at time T+DT of ion species A
AGAMk	array of length MAXZ in which the currents due to ion species A at gate k are stored
DA	total distance that the cell space for species A has drifted
DAR	radial diffusion coefficient for ion species A
DAZ	axial diffusion coefficient for ion species A
DNA	initial density of species A measured at the peak of the distribution
DR	grid size in the radial direction
DZ	grid size in the axial direction
DT	time step
E	electric field value (volts/cm)
EON	ratio of electric field to gas number density (volts cm^2)
IAk	counter for storing the currents at gate k for ion species A
INGAk	switch which indicates when distribution A has passed gate k
Kk	represents the distance from leftmost cell of the cell space A to gate k (cell space assumed drifting from left to right)
Lk	represents the distance from the leftmost cell of the cell space C to gate k
Mk	represents the distance from the leftmost cell of the cell space B to gate k
MAXAk	internal switch which indicates when the cell space for species A is traversing gate k

MAXZ	number of cells in the axial direction
P1	pressure of the reactant gas through which the ions are drifting (Torr)
P2	pressure of the buffer gas through which the ions are drifting (Torr)
RAB	frequency of the reaction producing ion species A from ion species B
RO	Gaussian halfwidth in radial direction of initial ion species distributions
SING	indicates whether rescaling is necessary for species A in the radial or axial direction
T	total drift time
TAk	array of length MAXZ containing corresponding times for AGAMk
TEMP	temperature of the system
TING	indicates whether rescaling is necessary for species B in the radial or axial direction
VA	drift velocity of ion species A
XKA	mobility of ion species A
XKOA	reduced mobility of ion species A
XLk	position of gate k
XN1	density of gas 1
XN2	density of gas 2
YKAB	rate constant for ion species A converting to B
ZING	indicates whether rescaling is necessary for ion species C in the radial or axial direction
ZO	full Gaussian width in the axial direction of the inital ion species distribution

I. INTRODUCTION

The performance of communications systems, radars, and other defense systems are often predicted using phenomenology codes, some of which employ simplified chemistry. Extensive chemical codes of the lower ionosphere are being used to check the reliability of the simplified chemistry. The development of these large chemical codes requires both *in situ* measurements of ionic- and neutral-constituent number densities and laboratory measurements of the relevant reaction rate constants. One of the laboratory tools that is particularly well suited for studying ion-molecule reactions is the drift tube. One of these is now in operation at the Ballistic Research Laboratories (BRL).

A typical drift tube configuration is shown in Figure 1. Ions are produced in the ion source. An axial electric field causes them to drift down the tube, and most of them impact the end wall. Some of the ions are swept through the exit aperture into the mass spectrometer. Typically the source runs continuously, with one of the pairs of electrical grids, called "shutters," serving as the point of origin for a swarm of ions. That shutter, the "starting shutter," is electrically biased to stop the drift of ions; then it is opened by applying a pulse of dc voltage for a few microseconds to allow a spatially small group of ions to start down the tube. As the cloud of ions drifts, it diffuses both axially and radially, and the ions react with the gas molecules in the tube to form other ions which have their own drift velocities and diffusion coefficients. The mass spectrometer is used to select ions of one mass number from the ions that emerge from the exit aperture, and the signals due to the arrival of ions of that mass are sorted and stored in a multichannel analyzer as a function of the time since the starting shutter was pulsed on. Typically, fewer than one ion per ion group negotiates the drift tube and mass analysis chamber and is counted, so that the starting shutter must be pulsed many times before statistically significant arrival time profiles for the several ions are accumulated. A complete set of these profiles for two gas pressures at a convenient value of E/N, where E is the drift field strength and N is the gas number density, contains

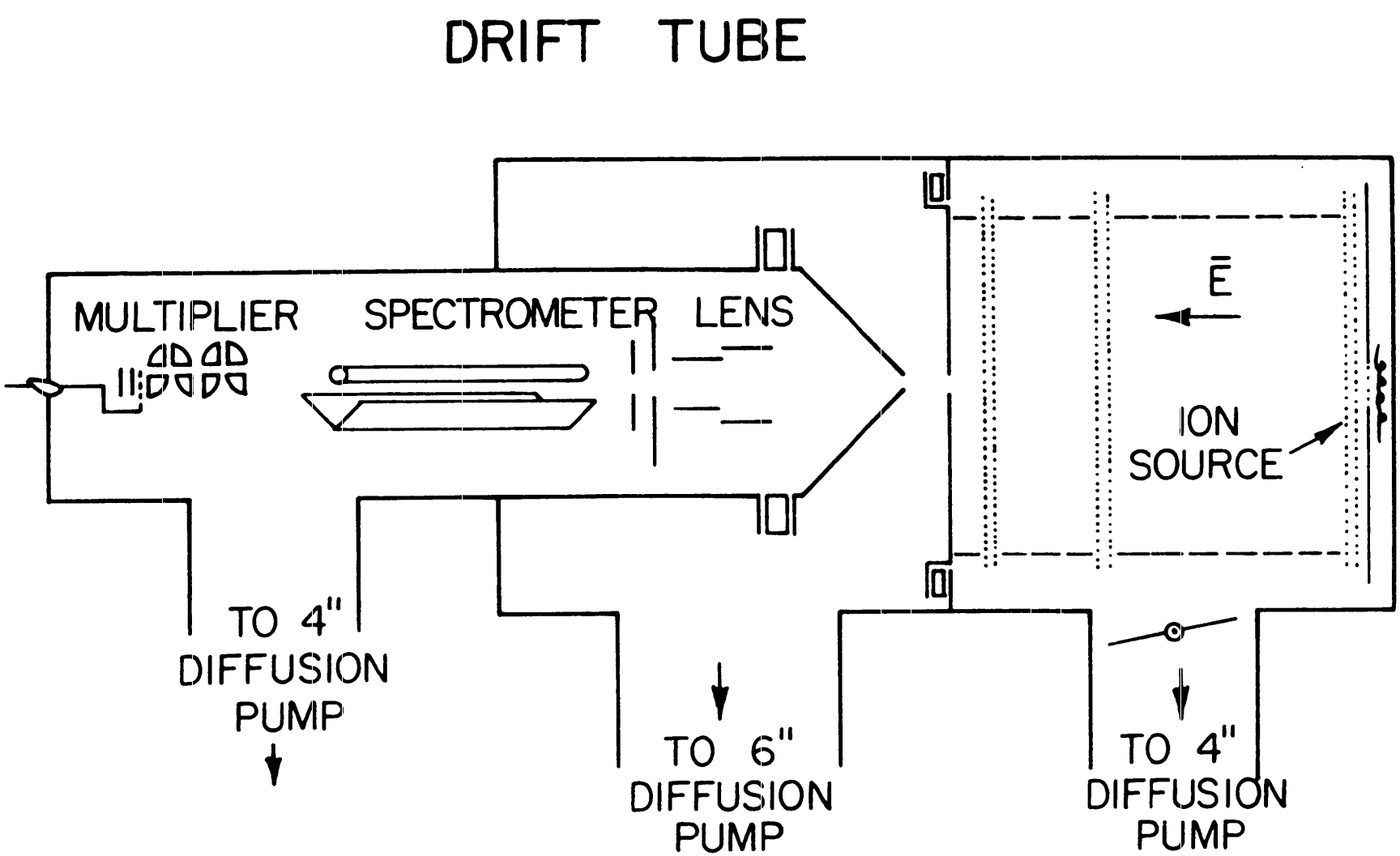

Figure 1. Typical Drift Tube Configuration

the information necessary to deduce the drift velocities (and thus mobilities) and the reaction rate constants. Unfortunately the rate constants and some of the drift velocities cannot be easily deduced from the arrival time curves. One approach is to compare measured arrival time curves with curves calculated for a variety of parameters to insure that the desired physical quantities are uniquely determined. In generating the calculated arrival time curves one must take into account all the known physical phenomena which will affect the shapes of the curves, including all possible reactions of all emerging ions. A computer program, MULTIGATE, has been developed at the BRL which permits numerical modeling of the drift, diffusion, and reactions of several ions in a drift tube.

MULTIGATE is a FORTRAN IV program, originally conceived of by Kregel, that uses an iterative numerical technique for drift tube modeling. MULTIGATE uses finite difference calculus to generate time arrival histories at several points, or "gates," in the drift space for several ionic species. The modified Euler method is employed for performing the actual numerical integration phase of the program. At present, the program is written for - though not limited to - three ion species and four intermediate gates, and one end gate, hence the name MULTIGATE.

In the program finite cylindrical geometry (r,z) is assumed with the drift space divided into four concentric shells of equal thichness DR which are each in turn subdivided along Z into sections of length DZ. Ion densities are defined at the center of each of the resulting "rings" and are assumed to vary linearly between the centers. Each ring defines a cell for computational purposes. It has been found that 63 divisions along the z axis (making a total of 252 cells in all for each species) are adequate to effect a reasonable compromise between truncation error and computational time. The number of cells in the cell space for each ion is arbitrary provided that it is sufficiently large. One unique feature of the program which allows a significant reduction in the number of cells required is to have the cell space for each ion "drift" with the drift velocity of the corresponding ion species. This permits the peak of each ion cloud to remain more or less centered in its corresponding cell space.

II. MAIN PROGRAM

The primary purpose of the main program is to control the flow of computation and to control all output. It initially sets the limiting values of the variables, determines the size of each cell, sets the gate distances, and generates an initial distribution for each ion species in the appropriate cell spaces. At the beginning of each run, the following parameters are initialized:

Symbol Used in the Program	Symbol Definitions
XKOA, XKOB, XKOC	The reduced mobilities of ion species A, B, and C, respectively ($cm^2V^{-1}sec^{-1}$).
DNA, DNB, DNC	Initial densities of species A, B, and C measured at the peak of the distribution.
ZO, RO, XL	Full Gaussian width of the initial ion distributions in the axial direction, the Gaussian half width of the initial ion distributions in the radial direction, and total length of drift space (initially, the ion distributions are centered at Z=0 and later drift to Z=XL).
P1, P2, TEMP, EON	Pressure of the reactant gas through which the ions are drifting (Torr), pressure of the buffer gas, temperature of the gases (K) (assumed equal), and ratio of electric field to total gas number density (Vcm^2).
YKAB	Rate constant for reaction which forms B from A, or "A → B."
YKBA, YKAC, YKCA, YKBC, YKCB	Rate constants for reactions B → A, A → C, C → A, B → C, and C → B.

The main program also sets certain internal switches and counters used in the various subroutines to determine the state of the computation (defined below for gate 1):

MAXA1, MAXB1, MAXC1	Internal switches for indicating when the cell space for species A, B, and C, respectively, is traversing gate 1.
IAA1, IBB1, ICC1	Counters used to indicate where the values for the currents and corresponding times for ion species A, B, and C, respectively, are stored.

INGA1, INGB1, INGC1	Internal switches for indicating when the cell spaces for species A, B, and C, respectively, have traversed gate 1.
K1, M1, L1	Counters used to indicate the position (in units of cell thickness) of gate 1 with respect to the cell spaces for species A, B, and C, respectively.

The program contains similar internal switches and counters for the last four gates.

III. SELECTION OF DT

Throughout the computation the time step, DT, used in the integration of the ion densities is maintained at each time step at a value that will assure stability and minimize run time.

The maximum time step permitted by diffusion for each of the three ion species is computed by the following method. The particle current density $\bar{J}$ due to diffusion is defined vectorially as

$$\bar{J} \equiv -D\nabla n \tag{1}$$

where D is the diffusion coefficient and n is the particle number density. Since cylindrical symmetry is assumed in our case, $\bar{J}$ may be approximated using finite difference calculus as

$$\bar{J} \approx -D_z \frac{\Delta n}{\Delta z} \bar{i}_z - D_r \frac{\Delta n}{\Delta r} \bar{i}_r \tag{2}$$

$$\approx J_z \bar{i}_z + J_r \bar{i}_r \ , \tag{3}$$

in which $\bar{i}_z$ and $\bar{i}_r$ are unit vectors in the z and r direction, respectively, and Δn, Δr, and Δz are finite differences denoting differences in density, in distance in the $\bar{i}_r$ direction and in distance in the $\bar{i}_z$ direction, respectively.

In the following discussion we shall consider a cell of thickness Δr and length Δz located at r_o and z_o. From the continuity equation (also cast into a finite difference equation) we know that the particle

current density evaluated at a particular surface of a cell times the surface area summed over all cell surfaces when divided by the cell volume will approximate the negative of the time rate of change of the density, n, in that cell. Current is defined to be positive if it is directed in the direction of the appropriate unit vector. Thus the instantaneous time derivative of n may be written as

$$-\frac{dn}{dt} \approx \frac{-A(z_o)\ J_z(z_o) + A(z_o + \Delta z)\ J_z(z_o + \Delta z) - A(r_o)\ J_r(r_o) + A(r_o + \Delta r)\ J_r(r_o + \Delta r)}{2\pi r_o \Delta r \Delta z}, \tag{4}$$

where $A(z_o)$ and $J_z(z_o)$ denote the cell area defined by the surface for which $z = z_o$, $r_o \leq r \leq r_o + \Delta r$ and the current through that surface, respectively, and where the other areas and currents are defined in a similar manner. All areas are assumed to be positive in extent.

We shall let Δn denote the amount by which the ion number density in the cell differs from the "average" density in each of the surrounding cells, and shall assume that

$$J_z(z_o) \approx -J_z(z_o + \Delta z) \equiv -D_z \frac{\Delta n}{\Delta z}$$

and

$$J_r(r_o) \approx -J_r(r_o + \Delta r) \equiv -D_r \frac{\Delta n}{\Delta r}.$$

Substitution yields

$$-\frac{dn}{dt} \approx \frac{D_z\left[A(z_o) + A(z_o + \Delta z)\right]\frac{\Delta n}{\Delta z} + D_r\left[A(r_o) + A(r_o + \Delta r)\right]\frac{\Delta n}{\Delta r}}{2\pi r_o \Delta r \Delta z}. \tag{5}$$

If

$$A(z_o) \approx A(z_o + \Delta z) \approx 2\pi r_o \Delta r$$

and if

$$A(r_o) \approx A(r_o + \Delta r) \approx 2\pi r_o \Delta z,$$

then,

$$-\frac{dn}{dt} \approx 2\,\frac{D_z \Delta n}{\Delta z^2} + 2\,\frac{D_r \Delta n}{\Delta r^2} \,. \tag{6}$$

Equation (6) emphasizes the fact that if Δn is positive, the time rate of change of the ion number density is negative; that is, there is a net loss of ions from the cell. If Δn is assumed to vary linearly in time in the interval Δt and if coupling between the densities in the other cells is neglected, the time increment associated with a change of Δn in the density in a cell can be expressed, in terms of finite differences, as

$$\Delta t \approx \frac{1}{2}\left(\frac{D_r}{\Delta r^2} + \frac{D_z}{\Delta z^2}\right)^{-1} \,. \tag{7}$$

Limiting Δt then limits the possible Δn in any one time step. To insure stability of the solution, Δt is set to 0.75 times this value in order to damp out any "noise" on n.

Current calculations take place as cells drift a distance XL in the x-direction, that is, as they pass the imaginary end plate. Consideration must be made of the effects of the distance that each cell space drifts during a single time step. If the time step were so large that a cell space drifted a distance equal to several DZ, there would be fewer current calculations than there were axial cells for that ion, thus diminishing the desired output of the program. Therefore we calculate the *maximum* size of the time step permitted by the drift velocities of the ions by the formula

$$\Delta t = \frac{g \times DZ}{v_{max}} \,, \tag{8}$$

where v_{max} is the drift velocity of the fastest ion, g is a control factor equal to the number of cells which may drift past the end plate in one time step, and DZ is the axial grid size. This procedure insures that there will be about MAXZ/g current calculations for the fastest ion. We usually set g = 1.5.

Associated with each reaction is a rate constant, e.g., YKAB, and a frequency of reaction, e.g., RAB. The quantity 1.0/RAB is the time constant for the reaction whose rate constant is YKAB. The Δt for this reaction is set at $0.8 \times 1.0/RAB$, again to insure stability of the solution.

The program sets DT equal to the minimum time step calculated for diffusion, drift, or any of the reactions.

IV. INITIAL DISTRIBUTION

Initially the program assumes Gaussian distributions in both the radial and axial directions for the densities of all of the ion species. The distribution of ion species A is calculated from the relationship:

$$A(r,z) = DNA \times EXP\left[-\alpha r^2 - \beta(z - z_o)^2\right] , \tag{9}$$

where DNA is the initial value of A(r,z) at the peak of the distribution, α is calculated by the program from RO, the Gaussian halfwidth in the radial direction, to make the density in the fourth radial zone approximately 1/e its value at the center, and β is calculated from ZO, the full Gaussian width in the axial direction, to make the full width of the density profile in the longitudinal direction approximately ten cells. The parameter ZO insures that the initial distribution is centered in the cell space. The program then initializes the distributions for ion species B and C according to

$$B(r,z) = A(r,z) \times DNB/DNA \tag{10}$$

and

$$C(r,z) = A(r,z) \times DNC/DNA , \tag{11}$$

so that all species have initially the same distribution shapes.

V. DERIVATIVE SUBROUTINE - S

Subroutine S is used to calculate time derivatives of the ion number densities and of predicted ion number densities in the cells in the three inner radial shells. Effects of drift, diffusion, and chemistry are handled in S.

The calculation begins by approximating the current density at the four boundaries of each cell using second order difference calculus. These four current densities are then multiplied by the corresponding incremental areas and summed. This resulting sum is then divided by the incremental volume of the corresponding cell to yield the time rate of change of density due to diffusion. Effects of mobility are taken into account automatically since the cells are allowed to "drift" with the drift velocity of the corresponding ionic species.

The time rate of change of the density due to chemistry for each ionic species at each cell is easily calculated by multiplying the rate constants by the appropriate densities of the interacting ionic species evaluated at the center of that cell. First order extrapolation techniques are used for this.

Thus, in generating the derivatives due to diffusion the subroutine calculates the current densities times the incremental area in consecutive cells in the radial and axial directions. The following names are used in subroutine S:

HA's	Represent densities of A.
GA's	Denote product of current density and area or the number of ions/sec passing through an elementary area.
HAP	Density of A in cell (j=1,2,3, or 4; k=1,2,3,..., or MAXZ).
HA	Density of A in cell (j,k+1), in increasing axial direction.
HAR	Density of A in cell (j+1,k), in increasing radial direction.
GAZP	Current flowing into cell (j,k) in axial direction.
GAZ	Current flowing out of cell (j,k) in axial direction.
GARP	Current flowing into cell (j,k) in radial direction.
GAR	Current flowing out of cell (j,k) in radial direction.

In addition to the ion diffusion, the program must also calculate the effects of chemical reactions upon the three ions. Since the cell spaces of the three ions, in general, do not drift at the same speed, the program must keep track of the relative shift of the cell spaces in order

to "bring together" the points of equal drift distance of the three ions. To accomplish this, the main program records the drift distances of the three cell spaces in DA, DB, and DC. Each drift distance is, of course, the sum over time of the corresponding drift velocity times the appropriate time step.

VI. SCALING - BANGR, RAP, BANGZ, AND ZAP

During the calculation, tests are made each time step to determine whether rescaling is necessary in either the radial or axial direction. The subroutine BANGR is used to determine whether rescaling is necessary in the radial direction. Since the ion distributions tend to remain centered in their respective cell spaces, it is only necessary to test in a plane perpendicular to the axis halfway down the cell space of each ion. Rescaling in the radial direction occurs only when, for any ion species, the ratio of the density in the cell in the outer radial shell to the cell in the innermost shell is greater than 0.9, a number chosen by trial and error. Number densities corresponding to an expanded radial grid are calculated in subroutine RAP.

To determine whether axial rescaling is necessary, densities in the cells in the innermost radial shells are tested in BANGZ. The sum of the densities in the first six cells, SUMA, and the sum of the densities in the last six cells, SUMB, are compared with the sum of the densities in all the inner cells, SUMC. If one of the ratios SUMA/SUMC or SUMB/SUMC is greater than 0.00001 and the other is greater than 0.000005, rescaling of the axial cells by a factor of 2 is called for. If, however, one ratio is greater than 0.00001 while the other is less than 0.000005, indicating that the ion cloud is leaving the cell space at one end because of chemistry, the number densities are shifted by one cell to reduce the problem. If rescaling of the cell space has been called for, due to diffusion or chemistry, the new number densities, corresponding to an expanded axial grid, are calculated in subroutine ZAP. The main program suppresses axial rescaling if the center of the cell space of the most slowly drifting ion has drifted a distance greater than the length of the drift tube.

VII. INTEGRATION OF PREDICTOR-CORRECTOR METHOD USING CAL1, CAL2, AND S

Calculation of number densities in the cell space of each ion begins at T = 0 with the initial values mentioned in Section IV. For convenience we shall describe the process only for species A. The appropriate DT is computed, and the time counter, T, is incremented by this factor. The first application of subroutine S in each iteration computes the time derivative of the initial number density, A, for all cells in the three inner radial shells and stores these values in AP. Then CAL1 uses A and AP to compute the predicted value of the number density at time T, denoted by PA, in all cells in the three inner radial shells by the first order Euler method

$$PA = A + AP \times DT \ . \tag{12}$$

CAL1 assumes that the radial distribution of any ion at any axial position is Gaussian in order to compute PA for cells in the outer radial shell. The technique uses the PA's for the three cells directly inside that outer cell and a relation linking segments of a Gaussian distribution, as follows:

$$AP(\text{cell } 4) = AP^2(\text{cell } 3)/AP(\text{cell } 1) \ , \tag{13}$$

where the inner cell is cell 1 and the outer cell is cell 4. The time derivative of the predicted value of A is next calculated by S for all cells in the three inner radial shells, and the values are placed in APP. Finally, CAL2 calculates the value of A at the time T, replacing the old value of A. For cells in the three inner radial shells the second order Euler method is used.

$$A = A + (1/2)*(APP + AP)*DT \ , \tag{14}$$

where we have written a FORTRAN statement defining A over the time interval DT. For cells in the outer radial shell, the new A is also calculated assuming Gaussian radial distributions by the formula

$$A(\text{cell } 4) = A^2(\text{cell } 3)/A(\text{cell } 1) \ . \tag{15}$$

At this time BANGR and BANGZ test for the need for rescaling, and RAP and ZAP are used for this purpose as needed. A new DT is calculated, T is advanced, and calculations begin again at S.

VIII. CURRENT CALCULATION - CURNT

In subroutine CURNT, the currents reaching each gate are calculated and stored in AGAM, BGAM, and CGAM, etc. The routine determines the position of the gate in each cell space and calculates the current from the densities of the two adjoining cells which straddle the gate at the time T. That is, the value is calculated according to the formula

$$\Gamma_z = -D_z \frac{\Delta n}{\Delta z} + v_z \times n \ , \qquad (16)$$

where Γ_z, D_z, $\Delta n/\Delta z$, and v_z are the values at the gate of the current, diffusion coefficient, space rate of change of number density, and drift velocity, respectively, in the axial direction, and n is the number density at the gate. The value of n in Equation (16) is determined by linear interpolation. If all of the cells in the cell space have passed the gate, the calculation of the current is terminated for that ion at that particular gate. When the cell spaces for ions A, B, and C have all passed the final gate, the entire calculation is stopped and the program prints output values.

IX. EFFECT OF CHANGING MAXZ

A comparison of results obtained from running the code for differing values of MAXZ is shown in Figure 2. The initial parameters of the calculation are shown on the figure. The use of MAXZ = 63 or greater is seen to produce essentially identical results, except that the use of larger values of MAXZ yields more data points on the arrival time curve. The run time for the code also increases as MAXZ increases, however.

X. COMPARISON WITH ANALYTICAL CODE

Woo and Whealton[1*] have developed a three-dimensional analytical model of a drift tube which considers drift, diffusion, and one reaction. Figure 3 shows a comparison of a calculation by their code to a calculation made using MULTIGATE, with the initial conditions for each calculation set as nearly identical as possible. The arrival curves were normalized to produce the same height peaks, but are otherwise unchanged. The agreement could be improved with a few-microsecond shift of the time

*References may be found on page 26.

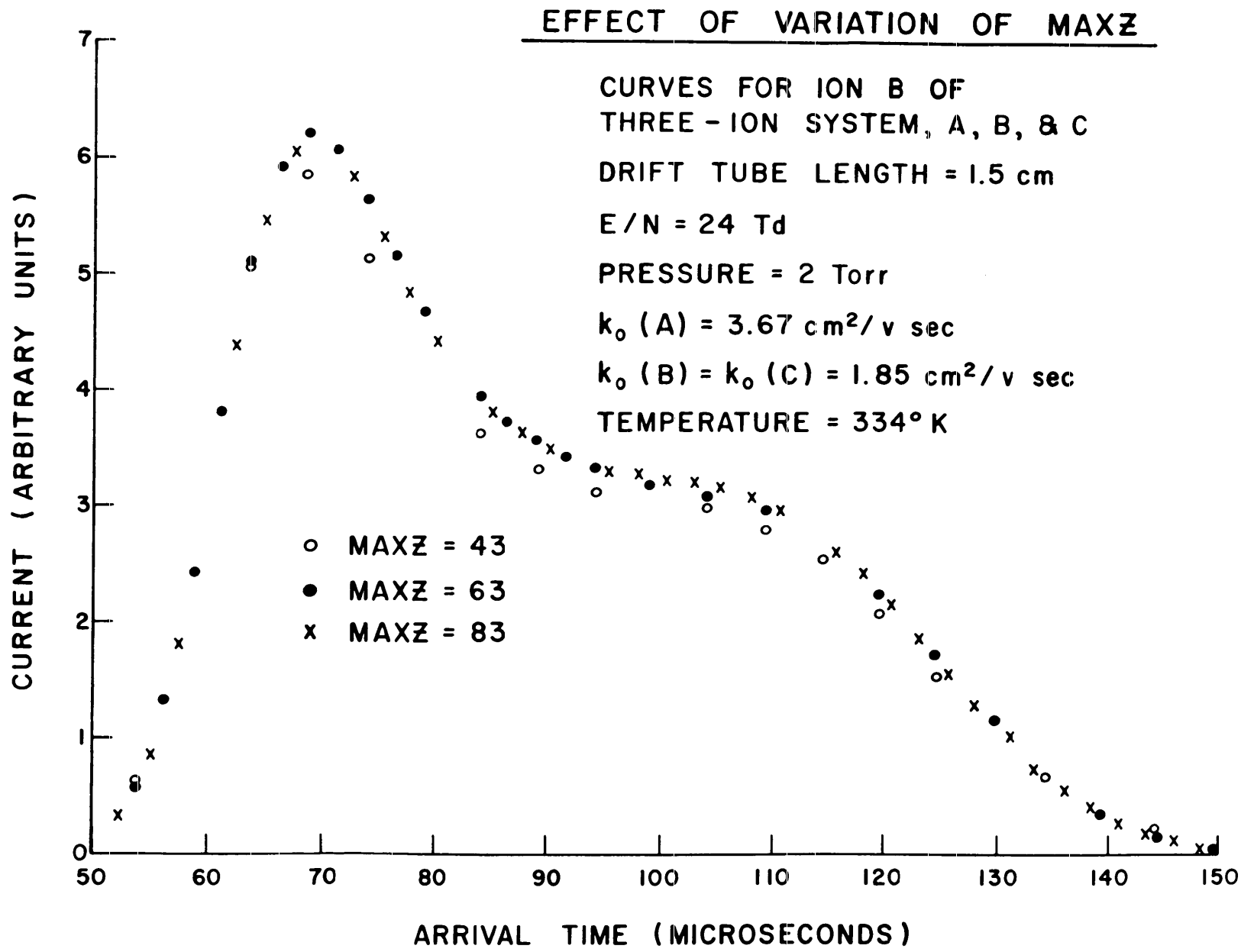

Figure 2. Comparison of Time Arrival Spectra for Varying Values of MAXZ

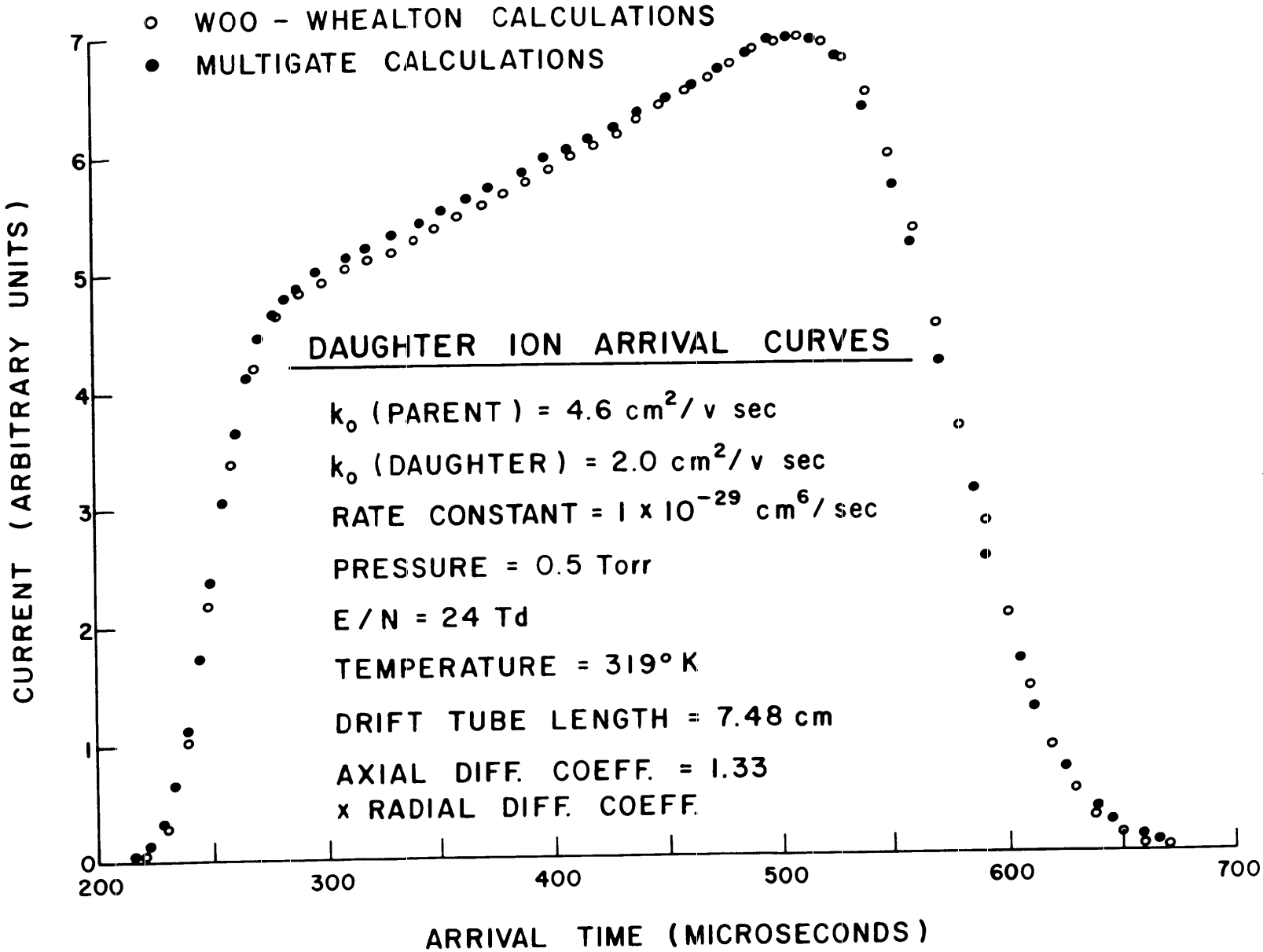

Figure 3. Comparison of Time Arrival Spectra Generated by Woo and Wealton's Analytical Code and by MULTIGATE Numerical Code

axis, but the curves are seen to be in agreement, in spite of the drastically different methods used to calculate them. It is not known if the shift disagreement is due to assumptions used in the analytical model or to truncation effects in the numerical model.

XI. SUBROUTINE PLOT

Subroutine PLOT was written to provide a rough plot of the three theoretical current distributions on a single computer output page. The height of each distribution is independently scaled with ordinate values referring to ion A only.

PLOT uses two other subroutines, SETUP and SORT.[2] SETUP is used in the Y-scaling and returns the minimum Y-value, the scale factor, and the width, defined as the maximum minus the minimum value. After scaling, points are plotted on a 50 × 120 grid using the letters, "A," "B," and "C." In the event that two points fall in the same position, a "D" is printed.

XII. SUMMARY

A FORTRAN IV program has been written which models ion transport and chemistry in a drift tube. While the program presented in this report is concerned with three ions, the program could be extended to four or more ions, if desired. Similarly, the program could accommodate any conceivable ion distribution at the beginning of the ion drift. The program can therefore be used to model the ion transport and chemistry of any conceivable drift tube experiment. It can also be used to check analytical drift tube models as well as to determine the conditions under which one-dimensional drift tube models, whether analytical or numerical, can be safely used.

REFERENCES

1. S.-B. Woo and J. H. Whealton, "Transport Model for Converting Charged Species in Drift Tubes," *Phys. Rev.* 180, 314 (1969).

2. For a description of SORT, see R. E. Funderlic, ed., The Programmer's Handbook, Union Carbide Corporation Report K-1729.

APPENDIX

LISTING OF PROGRAM WITH OUTPUT

A complete listing of the program and its output is reproduced on the following pages. This calculation took 3.4 min on the BRL computer; it could be expected to take somewhat less than 1 min on a CDC 6600 machine.

519141

```
*     SP151   GEORGE KELLER  394  X3335  MULTIGATE                    11

$     MAXO(5000)LINES
      DIMENSION A(412),AP(412),PA(412),TA(103),AGAM(412),APP(412)
      DIMENSION B(412),BP(412),PB(412),TB(103),BGAM(412),BPP(412)
      DIMENSION C(412),CP(412),PC(412),TC(103),CGAM(412),CPP(412)
      DIMENSION AGAM1(103),AGAM2(103),AGAM3(103),AGAM4(103)
      DIMENSION BGAM1(103),BGAM2(103),BGAM3(103),BGAM4(103)
      DIMENSION CGAM1(103),CGAM2(103),CGAM3(103),CGAM4(103)
      DIMENSION TA1(103),TA2(103),TA3(103),TA4(103)
      DIMENSION TB1(103),TB2(103),TB3(103),TB4(103)
      DIMENSION TC1(103),TC2(103),TC3(103),TC4(103)
      COMMON MAXZ,DR,DZ,DT,PI
      PI=3.1415926536
C REDUCED MOBILITY OF SPECIES A IN UNITS OF CM**2/V*SEC
      XK0A=3.67
C REDUCED MOBILITY OF SPECIES B IN UNITS OF CM**2/V*SEC
      XK0B=1.85
C REDUCED MOBILITY OF SPECIES C IN UNITS OF CM**2/V*SEC
      XK0C=1.85
C TOTAL DRIFT DISTANCE IN UNITS OF CM
      XL=7.5
C RADIUS OF INITIAL ION BURST IN RADIAL DIRECTION IN UNITS OF CM
      R0=.25
C LENGTH OF INITIAL ION BURST IN LONGITUDINAL DIRECTION IN UNITS OF CM
      Z0=.3
C INITIAL NUMBER DENSITY OF SPECIES A, IN ARBITRARY UNITS
      DNA=1.0E12
C INITIAL NUMBER DENSITY OF SPECIES B, IN ARBITRARY UNITS
      DNB=1.0
C INITIAL NUMBER DENSITY OF SPECIES C, IN ARBITRARY UNITS
      DNC=1.0
C GAS TEMPERATURE, IN UNITS OF DEGREES K
      TEMP=334.
C RATIO OF DRIFT FIELD TO GAS NUMBER DENSITY, IN UNITS OF V*CM*CM
      EON=24.E-17
C AS CURRENTLY SET UP, THIS PROGRAM ASSUMES  THAT THERE ARE TWO GASES IN THE
C DRIFT TUBE.  GAS TYPE 1 IS ASSUMED TO REACT WITH THE IONS, GAS TYPE 2 IS THE
C BUFFER GAS.  CHANGES TO SUIT OTHER CONDITIONS ARE STRAIGHTFORWARD.
C PRESSURE OF THE REACTANT GAS, IN UNITS OF TORR
      P1=2.0
C PRESSURE OF THE BUFFER GAS, IN UNITS OF TORR
      P2=0.0
C RATE CONSTANT FOR REACTION OF ION A TO FORM ION B , CM**6/SEC
      YKAB=2.8E-30
C RATE CONSTANT FOR REACTION OF ION B TO FORM ION A , CM**3/SEC
      YKBA=2.0E-14
C RATE CONSTANT FOR REACTION OF ION B TO FORM ION C , CM**6/SEC
      YKBC=1.2E-29
C RATE CONSTANT FOR REACTION OF ION C TO FORM ION B , CM**3/SEC
      YKCB=1.58E-13
      FAC=(3.54E16*273.0)/TEMP
      XN1=P1*FAC
      XN2=P2*FAC
      FACT=(P1+P2)*273.0/(760.0*TEMP)
      XKA=XK0A/FACT
      XKB=XK0B/FACT
      XKC=XK0C/FACT
      XNXN=XN1*(XN1+XN2)
C RAB IS THE FREQUENCY FOR REACTION OF ION A TO FORM ION B
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      RAB=YKAB*XNXN
      RBA=YKBA*(XN1+XN2)
      RBC=YKBC*XNXN
      RCB=YKCB*(XN1+XN2)
      RAC=0.0
      RCA=0.0
      E=EON*(XN1+XN2)
C THE VELOCITIES OF THE IONS
      VA=E*XKA
      VB=E*XKB
      VC=E*XKC
      FAC1=TEMP/1.16E4
      DAR=XKA*FAC1
      DBR=XKB*FAC1
      DCR=XKC*FAC1
C THE PROGRAM ASSUMES THAT THE R- AND Z-DIRECTION DIFFUSION COEFFICIENTS ARE
C EQUAL.   THE Z-DIRECTION COEFFICIENT CAN BE EXPECTED TO INCREASE AT HIGH
C VALUES OF E/N.
      DAZ=DAR
      DBZ=DBR
      DCZ=DCR
      DZ=ZO/30.0
      DR=RO/4.5
C PRINTING OF INPUT VALUES AND COMPUTED PARAMETERS.
      PRINT 201,   P1,P2
      PRINT 202,   YKAB ,YKBA
      PRINT 222,   YKBC ,YKCB
      PRINT 205,   ZO,RO,XL
      PRINT 206,   TEMP
      PRINT 207,   DNA,DNB,DNC
      PRINT 210,   XKOA,XKOB,XKOC
      PRINT 215,   E,EON
      PRINT 200,   VA,VB,VC
      PRINT 208,   DAR,DBR,DCR
      PRINT 209,   DAZ,DBZ,DCZ
      PRINT 211,   RAB,RBA
      PRINT 231,   RBC,RCB
      PRINT 214,   XN1,XN2
C SETTING OF INTERMEDIATE GATE POSITIONS.
      XL1=.2*XL
      XL2=.4*XL
      XL3=.6*XL
      XL4=.8*XL
      HZ=(ZO/2.0/DZ)**2
      HR=(RO/DR-0.5)**2
C N DETERMINES THE NUMBER OF CELLS IN THE Z-DIRECTION(MAXZ=2N+3).
      N=40
      MAXZ=N+N+3
      X=N+1
      III=1
      I=0
   37 IF(I.EQ.1) GO TO 10
C LIMITS DT TO MAX ALLOWED BY DIFFUSION OF SPECIES A
      DTAD=1.0/(DAZ/DZ**2+DAR/DR**2)/8.0*3.0
C LIMITS DT TO MAX ALLOWED BY DIFFUSION OF SPECIES B
      DTBD=1.0/(DBZ/DZ**2+DBR/DR**2)/8.0*3.0
C LIMITS DT TO MAX ALLOWED BY DIFFUSION OF SPECIES C
      DTCD=1.0/(DCZ/DZ**2+DCR/DR**2)/8.0*3.0
C  LIMITS DT TO MAX ALLOWED BY THE DRIFT VELOCITIES OF THE IONS
      DTV=1.5*DZ/(AMAX1(VA,VB,VC)+1.0)
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C  LIMITS DT TO MAX ALLOWED BY  REACTIONS AMONG THE SPECIES
      DTR=0.8*(1.0/AMAX1(RAB,RBA,RAC,RCA,RBC,RCB))
      DT=AMIN1(DTAD,DTBD,DTCD,DTV,DTR)
      IF(DT.EQ.DTR) I=1
   10 GO TO (38,40,41),III
C SWITCHES SET TO 0 INITIALLY
   38 MAXA=0
      MAXA1=0
      MAXA2=0
      MAXA3=0
      MAXA4=0
      MAXB=0
      MAXB1=0
      MAXB2=0
      MAXB3=0
      MAXB4=0
      MAXC=0
      MAXC1=0
      MAXC2=0
      MAXC3=0
      MAXC4=0
      L=0
      MB=0
      M1=0
      M2=0
      M3=0
      M4=0
      KA=0
      K1=0
      K2=0
      K3=0
      K4=0
      LC=0
      L1=0
      L2=0
      L3=0
      L4=0
      IAA=0
      IAA1=0
      IAA2=0
      IAA3=0
      IAA4=0
      IBB=0
      IBB1=0
      IBB2=0
      IBB3=0
      IBB4=0
      ICC=0
      ICC1=0
      ICC2=0
      ICC3=0
      ICC4=0
      INGA=0
      INGA1=0
      INGA2=0
      INGA3=0
      INGA4=0
      INGB=0
      INGB1=0
      INGB2=0
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      INGB3=0
      INGB4=0
      INGC=0
      INGC1=0
      INGC2=0
      INGC3=0
      INGC4=0
C SUMS INITIALLY SET TO 0
      AGAM(MAXZ)=0.0
      AGAM1(MAXZ)=0.0
      AGAM2(MAXZ)=0.0
      AGAM3(MAXZ)=0.0
      AGAM4(MAXZ)=0.0
      BGAM(MAXZ)=0.0
      BGAM1(MAXZ)=0.0
      BGAM2(MAXZ)=0.0
      BGAM3(MAXZ)=0.0
      BGAM4(MAXZ)=0.0
      CGAM(MAXZ)=0.0
      CGAM1(MAXZ)=0.0
      CGAM2(MAXZ)=0.0
      CGAM3(MAXZ)=0.0
      CGAM4(MAXZ)=0.0
C CALCULATION OF INITIAL DENSITY DISTRIBUTIONS.
      DO 6 K=1,4
      XK=K
      DO 6 J=1,MAXZ
      XJ=J
      L=L+1
      A(L)=EXP(-(XJ-X)**2/HZ-(XK-0.5)**2/HR)
      IF(J.EQ.1) A(L)=0.0
      C(L)=A(L)*DNC/DNA
    6 B(L)=A(L)*DNB/DNA
C DA,DB,DC REPRESENT TOTAL DISTANCE TRAVELED BY A,B,C.
      DA=0.0
      DB=0.0
      DC=0.0
      T=0.0
      DO 100 JKL=1,1000
      T=T+DT
      DA=DA+VA*DT
      DB=DB+VB*DT
      DC=DC+VC*DT
      L=0
C AP IS THE DERIVATIVE AT THE BEGINNING OF THE INTERVAL.
      CALL S(A,B,C,AP,DAZ,DAR,RAB,RBA,RAC,RCA,DA,DB,DC)
      CALL S(B,C,A,BP,DBZ,DBR,RBC,RCB,RBA,RAB,DB,DC,DA)
      CALL S(C,A,B,CP,DCZ,DCR,RCA,RAC,RCB,RBC,DC,DA,DB)
C C CAL1-FIRST-ORDER PREDICTOR SCHEME(PA,PB,PC-PREDICTED VALUES).
      CALL CAL1(A,AP,PA)
      CALL CAL1(B,BP,PB)
      CALL CAL1(C,CP,PC)
      CALL S(PA,PB,PC,APP,DAZ,DAR,RAB,RBA,RAC,RCA,DA,DB,DC)
      CALL S(PB,PC,PA,BPP,DBZ,DBR,RBC,RCB,RBA,RAB,DB,DC,DA)
      CALL S(PC,PA,PB,CPP,DCZ,DCR,RCA,RAC,RCB,RBC,DC,DA,DB)
C CAL2 SECOND ORDER CORRECTOR
      CALL CAL2(A,APP,AP)
      CALL CAL2(B,BPP,BP)
      CALL CAL2(C,CPP,CP)
C TEST FOR RADIAL RESCALING.
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      CALL BANGR(A,MAXZ,SING)
      CALL BANGR(B,MAXZ,TING)
      CALL BANGR(C,MAXZ,ZING)
      IF(SING+TING+ZING.EQ.0.0) GOTO 40
C A,B,C RESCALED IN R-DIRECTION BY RESETTING DR TO 1.1*DR.
      CALL RAP(A,MAXZ)
      CALL RAP(B,MAXZ)
      CALL RAP(C,MAXZ)
      DR=DR*1.1
      III=2
      GOTO 37
   40 CONTINUE
C TEST FOR Z RESCALING
      CALL BANGZ(A,MAXZ,SING,DA,DZ,KA)
      CALL BANGZ(B,MAXZ,TING,DB,DZ,MB)
      CALL BANGZ(C,MAXZ,ZING,DC,DZ,LC)
      IF(SING+TING+ZING.EQ.0.0) GOTO 41
C  IF SLOWEST ION HAS HAD CHANCE TO PASS OUT OF TUBE (NEGLECTING DIFFUSION),
C   STOP Z RESCALING
      IF(((AMIN1(VA,VB,VC))*T).GT.XL) GO TO 41
C A,B,C RESCALED IN Z-DIRECTION BY RESETTING DZ TO 2.0*DZ.
C IT IS ABSOLUTELY ESSENTIAL THAT THE FACTOR BY WHICH Z IS RESCALED BE LEFT AT 2
      CALL ZAP(A,MAXZ)
      CALL ZAP(B,MAXZ)
      CALL ZAP(C,MAXZ)
      DZ=DZ+DZ
      III=3
      GOTO 37
   41 CONTINUE
C CURRENTS CALCULATED AT 5 GATES FOR EACH SPECIES.
      CALL CURNT(A,MAXA,N,VA,T,XL,DAZ,TA,IAA,KA,AGAM,INGA,DA)
      CALL CURNT(A,MAXA1,N,VA,T,XL1,DAZ,TA1,IAA1,K1,AGAM1,INGA1,DA)
      CALL CURNT(A,MAXA2,N,VA,T,XL2,DAZ,TA2,IAA2,K2,AGAM2,INGA2,DA)
      CALL CURNT(A,MAXA3,N,VA,T,XL3,DAZ,TA3,IAA3,K3,AGAM3,INGA3,DA)
      CALL CURNT(A,MAXA4,N,VA,T,XL4,DAZ,TA4,IAA4,K4,AGAM4,INGA4,DA)
      CALL CURNT(B,MAXB,N,VB,T,XL,DBZ,TB,IBB,MB,BGAM,INGB,DB)
      CALL CURNT(B,MAXB1,N,VB,T,XL1,DBZ,TB1,IBB1,M1,BGAM1,INGB1,DB)
      CALL CURNT(B,MAXB2,N,VB,T,XL2,DBZ,TB2,IBB2,M2,BGAM2,INGB2,DB)
      CALL CURNT(B,MAXB3,N,VB,T,XL3,DBZ,TB3,IBB3,M3,BGAM3,INGB3,DB)
      CALL CURNT(B,MAXB4,N,VB,T,XL4,DBZ,TB4,IBB4,M4,BGAM4,INGB4,DB)
      CALL CURNT(C,MAXC,N,VC,T,XL,DCZ,TC,ICC,LC,CGAM,INGC,DC)
      CALL CURNT(C,MAXC1,N,VC,T,XL1,DCZ,TC1,ICC1,L1,CGAM1,INGC1,DC)
      CALL CURNT(C,MAXC2,N,VC,T,XL2,DCZ,TC2,ICC2,L2,CGAM2,INGC2,DC)
      CALL CURNT(C,MAXC3,N,VC,T,XL3,DCZ,TC3,ICC3,L3,CGAM3,INGC3,DC)
      CALL CURNT(C,MAXC4,N,VC,T,XL4,DCZ,TC4,ICC4,L4,CGAM4,INGC4,DC)
C TEST TO SEE WHETHER DISTRIBUTIONS HAVE PASSED THE LAST GATE.
C CALCULATION STOPS WHEN THE 3 DISTRIBUTIONS HAVE PASSED THE FINAL GATE.
      IF(INGA.EQ.1.AND.INGB.EQ.1.AND.INGC.EQ.1) GOTO 101
  100 CONTINUE
C OUTPUT VALUES PRINTED FOR FINAL AND 4 INTERMEDIATE GATES.
  101 CALL OUTP(AGAM1, TA1,BGAM1,TB1,CGAM1,TC1)
      CALL OUTP(AGAM2, TA2,BGAM2,TB2,CGAM2,TC2)
      CALL OUTP(AGAM3, TA3,BGAM3,TB3,CGAM3,TC3)
      CALL OUTP(AGAM4, TA4,BGAM4,TB4,CGAM4,TC4)
      CALL OUTP(AGAM,TA,BGAM,TB,CGAM,TC)
      STOP
  200 FORMAT(1H ,30X,3HVA=,1PE10.2,10X,3HVB=,1PE10.2,10X,3HVC=,1PE10.2)
  201 FORMAT(1H1,30X,3HP1=,F7.3,13X,3HP2=,F6.4)
  202 FORMAT(1H ,28X,5HYKAB=,1PE10.2,8X,5HYKBA=,1PE10.2)
  205 FORMAT(1H ,30X,3HZ0=,F6.4,14X,3HR0=,F6.4,14X,3HXL=,F9.5)
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  206 FORMAT(1H ,28X,5HTEMP=,F5.1)
  207 FORMAT(1H ,29X,4HDNA=,1PE10.2,9X,4HDNB=,1PE10.2,9X,4HDNC=,1PE10.2)
  208 FORMAT(1H ,29X,4HDAR=,1PE10.2,9X,4HDBR=,1PE10.2,9X,4HDCR=,1PE10.2)
  209 FORMAT(1H ,29X,4HDAZ=,1PE10.2,9X,4HDBZ=,1PE10.2,9X,4HDCZ=,1PE10.2)
  210 FORMAT(1H ,28X,5HXKOA=,F7.5,11X,5HXKOB=,F7.5,11X,5HXKOC=,F7.5)
  211 FORMAT(1H ,29X,4HRAB=,1PE10.2,9X,4HRBA=,1PE10.2)
  222 FORMAT(1H ,28X,5HYKBC=,1PE10.2,8X,5HYKCB=,1PE10.2)
  231 FORMAT(1H ,29X,4HRBC=,1PE10.2,9X,4HRCB=,1PE10.2)
  214 FORMAT(1H ,29X,4HXN1=,1PE10.2,9X,4HXN2=,1PE10.2)
  215 FORMAT(1H ,31X,2HE=,1PE10.2,9X,4HEON=,1PE10.2)
      END
C                                                                       BANGR
      SUBROUTINE BANGR(A,MAXZ,SING)
C BANGR DETERMINES WHETHER RESCALING IS NECESSARY IN THE R-DIRECTION.
      DIMENSION A(1)
C L-DESIGNATES INNER RADIAL ZONE.
      L=MAXZ/2
C K-DESIGNATES OUTER RADIAL ZONE.
      K=L+MAXZ+MAXZ+MAXZ
      SING=0.0
C RADIAL RESCALING CRITERIA.
      IF(A(K)/A(L).GT.0.90) SING=1.0
      RETURN
      END
C-                                                                      BANGZ
      SUBROUTINE BANGZ(A,MAXZ,SING,DA,DZ,IAP)
C BANGZ DETERMINES WHETHER RESCALING IS NECESSARY IN THE Z-DIRECTION.
C IF THE NEED OF Z RESCALING IS FOUND AT ONLY ONE END OF THE ION CLOUD, THE
C ENTIRE CLOUD IS SHIFTED ONE ZONE IN THE Z DIRECTION.
      DIMENSION A(1)
C SUMA-SUM OF DENSITIES IN 63 CELLS.
      SUMA=0.0
      DO 10  J=1,6
   10 SUMA=SUMA+A(J)
      SUMB=0.0
      MM6=MAXZ-6
      DO 20  J=MM6,MAXZ
   20 SUMB=SUMB+A(J)
      MM7=MM6-1
      SUMC=0.0
      DO 30  J=7,MM7
   30 SUMC=SUMC+A(J)
      SUMC=SUMC+SUMB+SUMA
      RATA=SUMA/SUMC
      RATB=SUMB/SUMC
      ISL=0
      ISR=0
      BZ=0.00001
      BZZ=0.000005
      IF(RATA.GT.BZ) ISL=1
      IF(RATB.GT.BZ) ISR=ISL+1
      SING=1.0
      IF(ISR.EQ.2) RETURN
      IF(ISL.EQ.0) GOTO 60
      MM=MAXZ-1
      IF(RATB.GT.BZZ) RETURN
      DO 50  K=1,4
      MMM=K*MAXZ
      DO 50  J=1,MM
      L=MMM-J
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   50 A(L+1)=A(L)
      IAP=IAP+1
      DA=DA-DZ
      SING=0.0
      RETURN
   60 IF(ISR.EQ.0) GOTO 90
      IF(RATA.GT.BZZ) RETURN
      MM=MAXZ-1
      DO 71  K=1,4
      MMM=MAXZ*(K-1)
      DO 70  J=2,MM
      L=J+MMM
   70 A(L)=A(L+1)
      MZ=K*MAXZ
   71 A(MZ)=A(MZ-1)/2.0
      IAP=IAP-1
      DA=DA+DZ
   90 SING=0.0
      RETURN
      END
C                                                                      CAL1
      SUBROUTINE CAL1(A,B,C)
C CAL1 IS A FIRST ORDER PREDICTOR SCHEME.
C A DENOTES THE INITIAL VALUE, B THE DERIVATIVE, AND C THE VALUE PREDICT
      DIMENSION A(1),B(1),C(1)
      COMMON MAXZ,DR,DZ,DT,PI
      L=0
      DO 10 K=1,3
      DO 10 J=1,MAXZ
      L=L+1
   10 C(L)=A(L)+B(L)*DT
      DO 30 J=2,MAXZ
      L1=J
      L3=MAXZ+MAXZ+J
      L4= L3+MAXZ
      C(L4)=0.0
   30 IF(C(L1).GT.1.0E-100) C(L4)=(C(L3)/C(L1))*C(L3)
      RETURN
      END
C                                                                      CAL2
      SUBROUTINE CAL2(A,B,C)
C CAL2 IS A SECOND ORDER CORRECTOR
      DIMENSION A(1),B(1),C(1)
      COMMON MAXZ,DR,DZ,DT,PI
      DTT=DT/2.0
      L=0
      DO 10 K=1,3
      DO 10 J=1,MAXZ
      L=L+1
   10 A(L)=A(L)+(B(L)+C(L))*DTT
      DO 30 J=2,MAXZ
      L1=J
      L3=MAXZ+MAXZ+J
      L4= L3+MAXZ
      A(L4)=0.0
   30 IF(A(L1).GT.1.0E-100) A(L4)=(A(L3)/A(L1))*A(L3)
      RETURN
      END
C                                                                      CURNT
      SUBROUTINE CURNT(A,MAX,N,VA,T,XL,DAZ,TA,IAA,IAP,AGAM,ING,DA)
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```
C CURNT GENERATES THE CURRENTS AT EACH GATE.
      DIMENSION A(1),TA(1),AGAM(1)
      COMMON MAXZ,DR,DZ,DT,PI
      IF(VA.EQ.0.0) RETURN
C ING=1 INDICATES THE DISTRIBUTION HAS PASSED THE GATE.
C IAA IS THE COUNTER FOR STORING THE CURRENTS AND CORRESPONDING TIMES IN
C THE AGAM AND TA ARRAYS RESPECTIVELY.
      IF(ING.EQ.1.OR.IAA.GE.MAXZ-1) GOTO 60
C XA IS THE DISTANCE FROM THE LEFTMOST CELL OF THE CELL SPACE TO THE GRI
      XA=(XL+FLOAT(N+1)*DZ-DA  )/DZ
      IA=XA
      ING=0
      IF(IA.GE.MAXZ) GOTO 50
      IF(MAX.EQ.0) IAA=0
      IF(MAX.EQ.0) IAP=0
      MAX=1
C TEST TO DETERMINE WHETHER DISTRIBUTION HAS PASSED THE GATE.
      IF(IA.LT.1)GOTO60
      L2=IA+MAXZ
      AL2=A(L2)
      AJ=A(IA)
      IF(AL2.GT.0.0.AND.AJ.GT.AL2) GOTO 40
      GOTO 70
   40 THE=XA-FLOAT(IA)
      OTHE=1.0-THE
      IX=IA
      AIA=AJ
      AIA1=A(IA+1)
      HOLD=OTHE*A(IX)+THE*A(IX+1)
      HOLD=-DAZ*(AIA1-AIA)/DZ+VA*HOLD
      AGAM(MAXZ)=AGAM(MAXZ)+HOLD*DT
      IF(IA.EQ.IAP)GOTO70
      IAP=IA
      IAA=IAA+1
      AGAM(IAA)=HOLD
      TA(IAA)=T
   50 RETURN
   60 ING=1
   70 RETURN
      END
C                                                                    INTER
      FUNCTION INTER(X)
C INTER INSURES ROUNDING DOWN IN ALL CASES
      INTER=(X+1000.0)
      INTER=INTER-1000
      RETURN
      END
C                                                                    OUTP
      SUBROUTINE OUTP(AGAM,TA,BGAM,TB,CGAM,TC)
C OUTP PRINTS THE OUTPUT VALUES.  OUTPUT CONSISTS OF CURRENTS AND CORRES
C PONDING TIMES FOR 3 IONS AT 5 GATES, AS WELL AS MEAN DRIFT TIMES, SUMS
C OF CURRENTS, AND RATIOS OF SUMS.
      DIMENSION AGAM(1),TA(1),BGAM(1),TB(1),CGAM(1),TC(1)
      COMMON MAXZ,DR,DZ,DT,PI
      COMMON /BAR/ T1,T2,T3
      PRINT 10
      DO 3  J=1,MAXZ
      IF(TA(J)+TB(J)+TC(J).EQ.0.0) GOTO 4
    3 PRINT 1, AGAM(J),TA(J),BGAM(J),TB(J),CGAM(J),TC(J)
    4 PRINT 5, AGAM(MAXZ)
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      PRINT 7, BGAM(MAXZ)
      PRINT 9, CGAM(MAXZ)
      T1=TBAR(AGAM,TA,SUM)
      T2=TBAR(BGAM,TB,SUM)
      T3=TBAR(CGAM,TC,SUM)
      PRINT 666, T1,T2,T3
      CALL PLOT(TA,AGAM,TB,BGAM,TC,CGAM)
      RETURN
    5 FORMAT(1H ,/,20X,5HSUMA=,1PE12.4)
    7 FORMAT(1H ,20X,5HSUMB=,1PE12.4)
    9 FORMAT(1H ,20X,5HSUMC=,1PE12.4)
    1 FORMAT(1H ,1P6E20.4)
   10 FORMAT(1H1,14X,1HA,17X,4HTIME,18X,1HB,17X,4HTIME,18X,1HC,17X,
     14HTIME)
  666 FORMAT(1H ,20X,3HTA=,1PE12.4,5X,3HTB=,1PE12.4,5X,3HTC=,1PE12.4)
      END
C                                                                      PLOT
      SUBROUTINE PLOT(X1,Y1,X2,Y2,X3,Y3)
C PLOT PLOTS 3 ION ARRIVAL SPECTRA VERSUS TIME. IT IS SET UP FOR 132 COL. PRINT
C MAGIC NUMBER 186 REFERS TO MAXIMUM NUMBERS OF CURRENT/TIME PAIRS
C MAGIC NUMBER 62 REFERS TO MAXIMUM NUMBER OF PAIRS PER ION SPECIES
      INTEGER BLANK,CA,CB,CC,CD
      DIMENSION X1(1),X2(1),X3(1),Y1(1),Y2(1),Y3(1)
      DIMENSION LINE(120),M(186),N(2,186),RMAN(6),RORD(13)
      DATA CA,CB,CC,CD,BLANK/1HA,1HB,1HC,1HD,1H /
      DATA LINE/120*1H /
      DO 2 I=1,186
      M(I)=0
    2 N(1,I)=0
      CALL SETUP(Y1,Y1S,Y1SC,Y1D)
      CALL SETUP(Y2,Y2S,Y2SC,Y2D)
      CALL SETUP(Y3,Y3S,Y3SC,Y3D)
      A=-1.E50
      B=1.E50
      L=0
      DO 6 I=1,62
      L=L+1
      N(1,L)=(Y1(I)-Y1S)*Y1SC+0.5
      N(2,L)=CA
      IF(N(1,L).EQ.0) GO TO 4
      XX=X1(I)
      IF(XX.GT.A) A=XX
      IF(XX.LT.B) B=XX
    4 L=L+1
      N(1,L)=(Y2(I)-Y2S)*Y2SC+0.5
      N(2,L)=CB
      IF(N(1,L).EQ.0) GO TO 5
      XX=X2(I)
      IF(XX.GT.A) A=XX
      IF(XX.LT.B) B=XX
    5 L=L+1
      N(1,L)=(Y3(I)-Y3S)*Y3SC+0.5
      N(2,L)=CC
      IF(N(1,L).EQ.0) GO TO 6
      XX=X3(I)
      IF(XX.GT.A) A=XX
      IF(XX.LT.B) B=XX
    6 CONTINUE
      X1D=A-B
      X1S=B-X1D/20.
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```
      X1D=X1D*1.1
C REPLACE 120 WITH 60 FOR 72 COLUMN OUTPUT
      X1SC=120./X1D
      L=0
      DO 7 I=1,62
      L=L+1
      M(L)=(X1(I)-X1S)*X1SC+0.5
      L=L+1
      M(L)=(X2(I)-X1S)*X1SC+0.5
      L=L+1
      M(L)=(X3(I)-X1S)*X1SC+0.5
    7 CONTINUE
      DO 8 I=1,186
      IF(N(1,I).GT.51) N(1,I)=N(1,I)-50
    8 N(1,I)=51-N(1,I)
      CALL SORT(M,N)
      DO 9 I=1,13
    9 RORD(I)=X1S+FLOAT(I-1)*X1D/12.
      DO 10 I=1,6
   10 RMAN(I)=Y1S+FLOAT(6-I)*Y1D/5.
      I=0
      LL=1
   11 I=I+1
      IF(N(1,I).NE.0) GO TO 12
      GO TO 11
   12 L=0
      PRINT 101
   13 L=L+1
      K=L-1
      KK=(K/10)*10
      IF(L.EQ.51) GO TO 20
   21 IF(M(I).NE.0) GO TO 22
      IF(I.GT.186) GO TO 23
      I=I+1
      GO TO 21
   22 IF(L.EQ.N(1,I)) GO TO 15
   23 IF(K.EQ.KK) GO TO 14
      PRINT 103
      GO TO 13
   14 PRINT 104, RMAN(LL)
      LL=LL+1
      GO TO 13
   15 J=M(I)
      JJ=LINE(J)
      LINE(J)=N(2,I)
      IF(JJ.NE.BLANK) LINE(J)=CO
      I=I+1
      IF(L.EQ.N(1,I)) GO TO 15
      IF(K.EQ.KK) GO TO 17
C REPLACE 120 WITH 60 FOR 72 COLUMN OUTPUT
      PRINT 106, (LINE(J),J=1,120)
      GO TO 18
C REPLACE 120 WITH 60 FOR 72 COLUMN OUTPUT
   17 PRINT 105,RMAN(LL),(LINE(J),J=1,120)
      LL=LL+1
   18 DO 19 J=1,120
   19 LINE(J)=BLANK
      GO TO 13
   20 PRINT 102,RMAN(LL),(RORD(J),J=1,13)
      RETURN
```

```
  101 FORMAT(57H1THEORETICAL CURVES - THE Y AXIS APPLIES TO ION SPECIES
     1A)
  102 FORMAT(E9.2,12(10H+---------),1H+,/,3X,13E10.2)
  103 FORMAT(9X,1HI)
  104 FORMAT(E9.2,1H+)
  105 FORMAT(E9.2,1H+,120A1)
  106 FORMAT(9X,1HI,120A1)
      END
C                                                                      RAP
      SUBROUTINE RAP(A,MAXZ)
C RAP RESCALES DENSITIES IN THE R DIRECTION.
      DIMENSION A(1)
      DO 58 J=2,MAXZ
      L2=J+MAXZ
      L3=L2+MAXZ
      L4=L3+MAXZ
      AJ=A(J)
      AL3=A(L3)
      IF(AL3.GT.0.0.AND.AJ.GT.AL3) GOTO 56
      A(J)=0.0
      A(L2)=0.0
      A(L3)=0.0
      A(L4)=0.0
      GOTO 58
   56 ALP=ALOG(AJ/AL3)/24.0
      DO 55 K=1,4
      L4=J+(K-1)*MAXZ
      HA=1.21*FLOAT(K+K-1)**2 -1.0
   55 A(L4)=AJ*EXP(-ALP*HA)
   58 CONTINUE
      RETURN
      END
C                                                                      S
      SUBROUTINE  S(A,B,C,AP,DAZ,DAR,RAB,RBA,RAC,RCA,DA,DB,DC)
C S RETURNS THE DERIVATIVE IN AP
      DIMENSION A(1),AP(1),B(1),C(1),GAR(103),GARP(103)
      COMMON MAXZ,DR,DZ,DT,PI
C XLC MEASURES THE RELATIVE DISTANCE OF C FROM A IN UNITS OF DZ.
      XLC=(DA-DC)/DZ
      LPC=INTER(XLC)
      THEC=XLC-FLOAT(LPC)
C XLB MEASURES THE RELATIVE DISTANCE OF B FROM A IN UNITS OF DZ.
      XLB=(DA-DB)  /DZ
      LPB=INTER(XLB)
      THEB=XLB-FLOAT(LPB)
      OTHEB=1.0-THEB
      OTHEC=1.0-THEC
      L=1
      LR=MAXZ
      DO 12 K=1,3
      XK=K
      XKP=K+K-1
      TPKDZ=2.0*PI*XK*DZ
      ARA=PI*XKP*DR**2
      VOL=ARA*DZ
      DAZDA=DAZ/DZ*ARA
      DARTP=DAR*TPKDZ
      HAP=0.0
      GAZ=0.0
      DO 12 J=1,MAXZ
```

```
      LM1=L
      L=L+1
      LR=LR+1
      IF(K.GT.1) GOTO 10
      GAR(J)=0.0
   10 GAZP=GAZ
      HA=0.0
      IF(J.LT.MAXZ) HA=A(L)
      GAZ=-DAZDA*(HA-HAP)
      HAR=A(LR)
      GARP(J)=GAR(J)
      GAR(J)=-DARTP*(HAR-HAP)
      IF(J.EQ.1) GOTO 14
      JPB=J+LPB
      KPB=JPB+MAXZ*(K-1)
      JPC=J+LPC
      KPC=JPC+MAXZ*(K-1)
      R=RAB+RAC
      CHB=0.0
      IF(JPB.LT.MAXZ.AND.JPB.GT.0  ) CHB=RBA*(B(KPB)*OTHEB
     1+B(KPB+1)*THEB)
      CHC=0.0
      IF(JPC.LT.MAXZ.AND.JPC.GT.0  ) CHC=RCA*(C(KPC)*OTHEC
     1+C(KPC+1)*THEC)
      AP(LM1)=    -(HAP*R-CHB-CHC+(GAR(J)-GARP(J)+GAZ-GAZP)/VOL)
   14 CONTINUE
      HAP=HA
   12 CONTINUE
      RETURN
      END
C                                                                    SETUP
      SUBROUTINE SETUP(X,B,Y1SC,Y1D)
C SETUP DETERMINES SCALE FACTORS FOR PLOTTING DIFFERENT ION SPECIES
C MAGIC NUMBER 62 REFERS TO MAXIMUM NUMBER OF PAIRS PER ION SPECIES
      DIMENSION X(1)
      A=-1.E50
      B=1.E50
      DO 1 L=1,62
      XX=X(L)
      IF(XX.GT.A) A=XX
      IF(XX.LT.B) B=XX
    1 CONTINUE
      Y1D=A-B
      Y1SC=50.0/Y1D
      RETURN
      END
C                                                                    SORT
      SUBROUTINE SORT(M,N)
C SORT INTERSORTS CURRENT/TIME PAIRS PRIOR TO THEIR BEING PLOTTED
C MAGIC NUMBER 186 REFERS TO MAXIMUM NUMBERS OF CURRENT/TIME PAIRS
      DIMENSION M(186),N(2,186)
      MM=186
    1 MM=MM/2
      IF(MM.EQ.0) RETURN
      K=186-MM
      J=1
    2 I=J
    3 IM=I+MM
      IF(N(1,I).LE.N(1,IM)) GO TO 4
      IT=M(I)
```

```
      M(I)=M(IM)
      M(IM)=IT
      DO 5 L=1,2
      IT=N(L,I)
      N(L,I)=N(L,IM)
    5 N(L,IM)=IT
      I=I-MM
      IF(I.GE.1) GO TO 3
    4 J=J+1
      IF(J.GT.K) GO TO 1
      GO TO 2
      END
C                                                              TBAR
      FUNCTION TBAR(XN,TI,SUM)
C TBAR CALCULATES THE MEAN DRIFT TIME.
      DIMENSION XN(1),TI(1)
      COMMON MAXZ,DR,DZ,DT,PI
      M=MAXZ-1
      TBAR=0.0
      SUM=0.0
      DO 1 I=1,M
      SUM=SUM+XN(I)
    1 TBAR=XN(I)*TI(I)+TBAR
      TBAR=TBAR/SUM
      RETURN
      END
C                                                              ZAP
      SUBROUTINE ZAP(A,MAXZ)
C ZAP RESCALES DENSITIES IN THE Z DIRECTION.
      DIMENSION A(1),TA(200)
      DO 44 K=1,4
      DO 40 J=1,MAXZ
   40 TA(J)=0.0
      N=(MAXZ-3)/2
      L=N/2+1
      DO 42 J=2,MAXZ,2
      M=J+(K-1)*MAXZ+1
      L=L+1
   42 TA(L)=A(M)
      DO 44 J=1,MAXZ
      I=J+(K-1)*MAXZ
   44 A(I)=TA(J)
      RETURN
      END
*     LIST
*     DATA
```

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P1= 2.000	P2= .0000	
YKAB= 2.80E-30	YKBA= 2.00E-14	
YKBC= 1.20E-29	YKCB= 1.68E-13	
ZO= .3000	RO= .2500	XL= 7.50000
TEMP=334.0		
DNA= 1.00E 12	DNB= 1.00E 00	DNC= 1.00E 00
XKOA=3.67000	XKOB=1.85000	XKOC=1.85000
E= 1.39E 01	EON= 2.40E-16	
VA= 2.37E 04	VB= 1.19E 04	VC= 1.19E 04
DAR= 4.91E 01	DBR= 2.48E 01	DCR= 2.48E 01
DAZ= 4.91E 01	DBZ= 2.48E 01	DCZ= 2.48E 01
RAB= 9.38E 03	RBA= 1.16E 03	
RBC= 4.02E 04	RCB= 9.72E 03	
XN1= 5.79E 16	XN2= 0.00E 00	

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A	TIME	B	TIME	C	TIME
1.4626E-10	2.8483E-05	1.0703E-03	3.8611E-05	1.4187E-03	4.1143E-05
6.4097E-09	2.9749E-05	4.2011E-03	3.9877E-05	4.7757E-03	4.2409E-05
1.2068E-07	3.1015E-05	1.6471E-02	4.1143E-05	1.4810E-02	4.3674E-05
2.5800E-06	3.2281E-05	5.4638E-02	4.2409E-05	4.1835E-02	4.4940E-05
2.9160E-05	3.3547E-05	1.5916E-01	4.3674E-05	1.1390E-01	4.6206E-05
3.4199E-04	3.4813E-05	4.1591E-01	4.4940E-05	2.9656E-01	4.7472E-05
2.4735E-03	3.6079E-05	1.0312E 00	4.6206E-05	1.5964E 00	5.0004E-05
1.7308E-02	3.7345E-05	2.4718E 00	4.7472E-05	6.0181E 00	5.2536E-05
8.4264E-02	3.8611E-05	3.5162E 01	5.2536E-05	4.4354E 01	5.7600E-05
3.8108E-01	3.9877E-05	8.9064E 01	5.5068E-05	9.2358E 01	6.0132E-05
1.3249E 00	4.1143E-05	1.8080E 02	5.7600E-05	1.6424E 02	6.2663E-05
4.2595E 00	4.2409E-05	4.3986E 02	6.2663E-05	3.6627E 02	6.7727E-05
1.1447E 01	4.3674E-05	5.4591E 02	6.5195E-05	4.7742E 02	7.0259E-05
2.8971E 01	4.4940E-05	6.0304E 02	6.7727E-05	5.8323E 02	7.2791E-05
6.4955E 01	4.6206E-05	5.7761E 02	7.2791E-05	7.6407E 02	7.7855E-05
1.4465E 02	4.7472E-05	5.3081E 02	7.5323E-05	8.3870E 02	8.0386E-05
5.2214E 02	5.0004E-05	4.8299E 02	7.7855E-05	9.0476E 02	8.2918E-05
1.4318E 03	5.2536E-05	4.4109E 02	8.0386E-05	9.6381E 02	8.5450E-05
3.1407E 03	5.5068E-05	3.8269E 02	8.5450E-05	1.0652E 03	9.0514E-05
5.4105E 03	5.7600E-05	3.6382E 02	8.7982E-05	1.1088E 03	9.3046E-05
7.4944E 03	6.0132E-05	3.5011E 02	9.0514E-05	1.1481E 03	9.5578E-05
8.4007E 03	6.2663E-05	3.3385E 02	9.5578E-05	1.2086E 03	1.0064E-04
7.6289E 03	6.5195E-05	3.2902E 02	9.8109E-05	1.2270E 03	1.0317E-04
5.7358E 03	6.7727E-05	3.2531E 02	1.0064E-04	1.2355E 03	1.0570E-04
3.5693E 03	7.0259E-05	3.2152E 02	1.0317E-04	1.2284E 03	1.0824E-04
1.8688E 03	7.2791E-05	3.1630E 02	1.0570E-04	1.2012E 03	1.1077E-04
8.5307E 02	7.5323E-05	3.0907E 02	1.0824E-04	1.1553E 03	1.1330E-04
3.4273E 02	7.7855E-05	2.9919E 02	1.1077E-04	1.0905E 03	1.1583E-04
1.4176E 02	8.0386E-05	2.6581E 02	1.1583E-04	1.0032E 03	1.1836E-04
6.6627E 01	8.2918E-05	2.4297E 02	1.1836E-04	8.9635E 02	1.2090E-04
4.3179E 01	8.5450E-05	2.1694E 02	1.2090E-04	7.7989E 02	1.2343E-04
3.4048E 01	8.7982E-05	1.8803E 02	1.2343E-04	6.5805E 02	1.2596E-04
2.9567E 01	9.0514E-05	1.5808E 02	1.2596E-04	5.3607E 02	1.2849E-04
2.6313E 01	9.3046E-05	1.2902E 02	1.2849E-04	4.2376E 02	1.3102E-04
2.3519E 01	9.5578E-05	1.0166E 02	1.3102E-04	3.2367E 02	1.3356E-04
2.1238E 01	9.8109E-05	7.7188E 01	1.3356E-04	2.3720E 02	1.3609E-04
1.9086E 01	1.0064E-04	5.7268E 01	1.3609E-04	1.6695E 02	1.3862E-04
1.7092E 01	1.0317E-04	4.0907E 01	1.3862E-04	1.1610E 02	1.4115E-04
1.5211E 01	1.0570E-04	2.7907E 01	1.4115E-04	7.7249E 01	1.4368E-04
1.3421E 01	1.0824E-04	1.8242E 01	1.4368E-04	4.8765E 01	1.4621E-04
1.0070E 01	1.1330E-04	1.1980E 01	1.4621E-04	3.4971E 01	1.4875E-04
7.0829E 00	1.1836E-04	8.3748E 00	1.4875E-04	1.1636E 01	1.5381E-04
4.5815E 00	1.2343E-04	3.1993E 00	1.5381E-04	1.1616E 00	1.6394E-04
2.6874E 00	1.2849E-04	9.6378E-01	1.5887E-04	3.0250E-01	1.6900E-04
1.9861E 00	1.3102E-04	8.7843E-02	1.6900E-04	5.8353E-02	1.7407E-04
1.4119E 00	1.3356E-04	2.2052E-02	1.7407E-04	3.1301E-03	1.8419E-04
6.5823E-01	1.3862E-04	4.1154E-03	1.7913E-04	5.8187E-04	1.8926E-04
2.7275E-01	1.4368E-04	6.0329E-04	1.8419E-04	7.8297E-05	1.9432E-04
1.1866E-01	1.4875E-04	3.9463E-05	1.9432E-04	8.6709E-06	1.9938E-04
4.3639E-02	1.5381E-04	5.3080E-06	1.9938E-04	4.8076E-07	2.0951E-04
2.0870E-02	1.5887E-04	5.9012E-07	2.0445E-04	5.5078E-08	2.1457E-04
4.5758E-03	1.6394E-04	3.2823E-08	2.1457E-04	5.3659E-09	2.1964E-04
1.6152E-03	1.6900E-04	3.7935E-09	2.1964E-04	2.8329E-10	2.2977E-04
3.2076E-04	1.7407E-04	3.7257E-10	2.2470E-04	3.0415E-11	2.3483E-04
1.2307E-04	1.7913E-04	1.9613E-11	2.3483E-04	2.7965E-12	2.3989E-04
1.3195E-05	1.8419E-04	2.1286E-12	2.3989E-04	1.4394E-13	2.5002E-04
4.1083E-06	1.8926E-04	1.9755E-13	2.4496E-04	1.5062E-14	2.5508E-04
5.5811E-07	1.9432E-04	1.0113E-14	2.5508E-04	1.3460E-15	2.6015E-04
2.1183E-07	1.9938E-04	1.0706E-15	2.6015E-04	6.7789E-17	2.7028E-04

1.2748E-08	2.0445E-04	9.6560E-17	2.6521E-04	7.0511E-18	2.7534E-04
4.1694E-09	2.0951E-04	2.8470E-17	2.7028E-04	6.2143E-19	2.8040E-04
4.5919E-10	2.1457E-04	4.8256E-18	2.7534E-04	1.6966E-19	2.8547E-04
1.8008E-10	2.1964E-04	5.0784E-19	2.8040E-04	3.0269E-20	2.9053E-04

SUMA= 1.1928E-01
SUMB= 2.7298E-02
SUMC= 6.4306E-02
TA= 6.3261E-05 TB= 9.0324E-05 TC= 1.0303E-04

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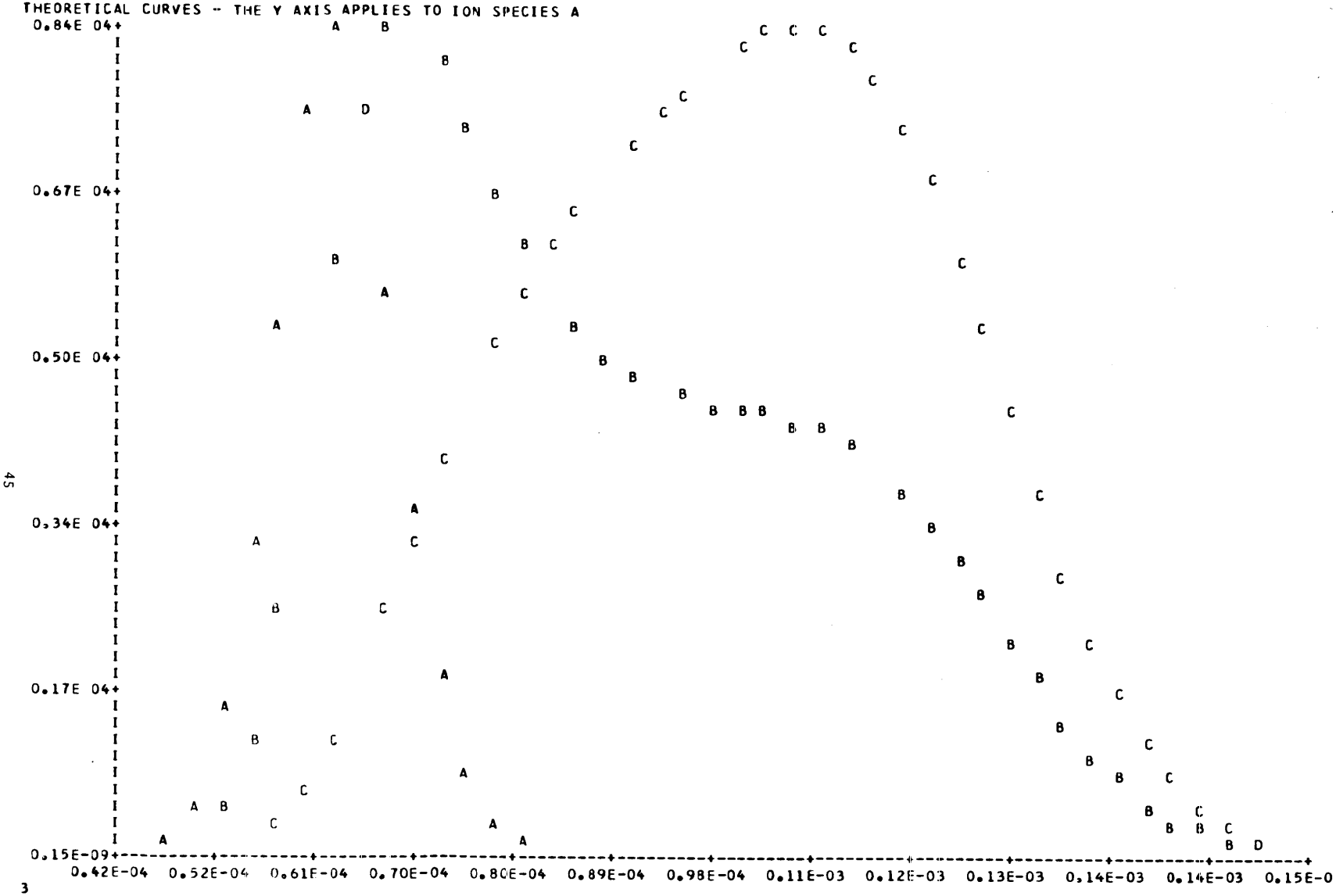
THEORETICAL CURVES -- THE Y AXIS APPLIES TO ION SPECIES A
0.84E 04
0.67E 04
0.50E 04
0.34E 04
0.17E 04
0.15E-09
0.42E-04
0.52E-04
0.61E-04
0.70E-04
0.80E-04
0.89E-04
0.98E-04
0.11E-03
0.12E-03
0.13E-03
0.14E-03
0.14E-03
0.15E-03

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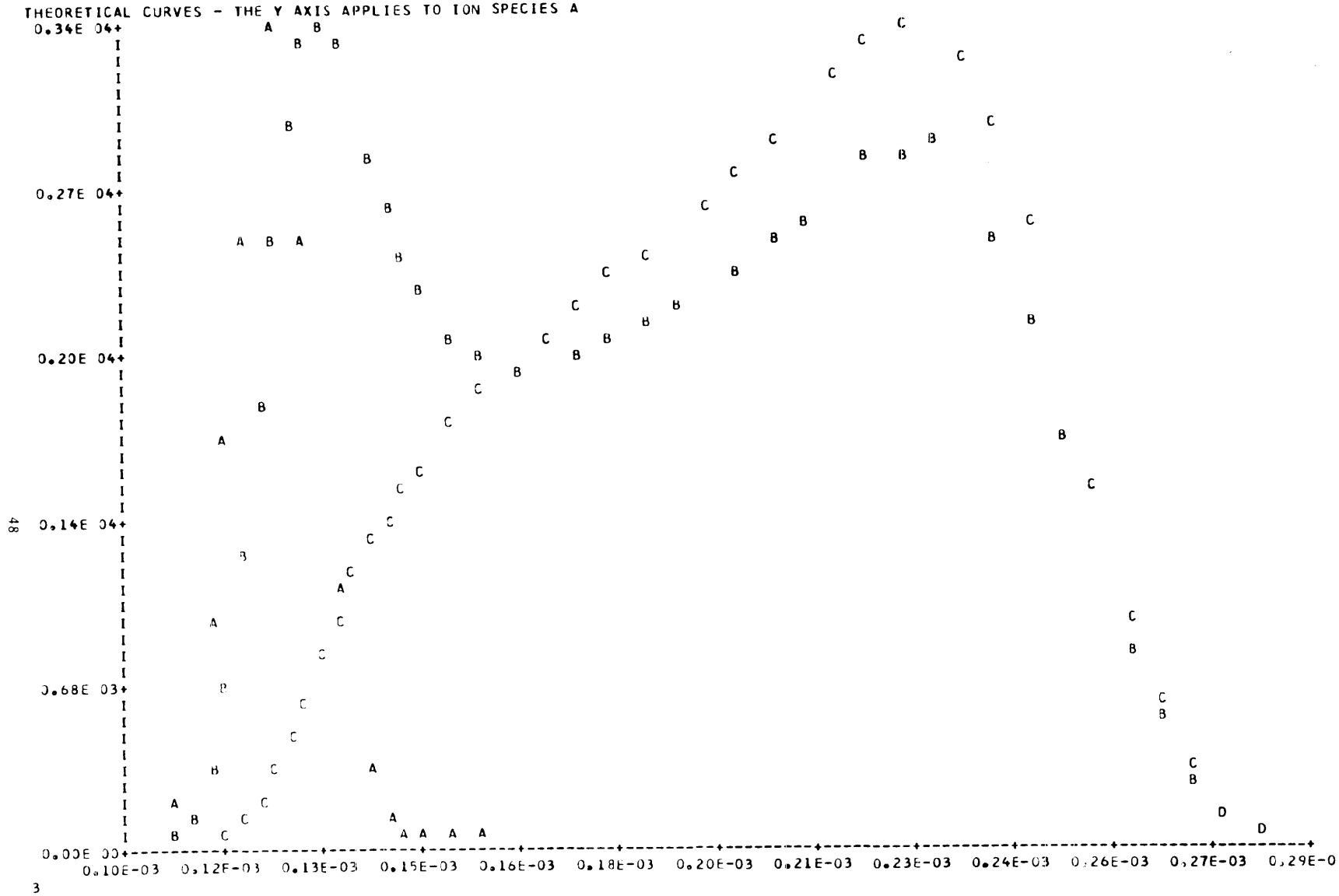
A	TIME	B	TIME	C	TIME
2.0717E-23	6.7727E-05	3.4811E-09	8.5450E-05	1.7836E-07	9.0514E-05
1.2268E-19	7.0259E-05	1.9842E-06	9.0514E-05	3.4884E-05	9.5578E-05
4.9350E-17	7.2791E-05	3.0382E-05	9.3046E-05	3.1252E-04	9.8109E-05
1.6449E-14	7.5323E-05	2.6449E-04	9.5578E-05	2.0779E-03	1.0064E-04
1.6499E-12	7.7855E-05	1.6797E-02	1.0064E-04	6.2644E-02	1.0570E-04
1.4756E-10	8.0386E-05	9.3130E-02	1.0317E-04	2.5623E-01	1.0824E-04
6.4797E-09	8.2918E-05	3.8304E-01	1.0570E-04	8.6213E-01	1.1077E-04
2.4476E-07	8.5450E-05	1.4299E 00	1.0824E-04	2.5698E 00	1.1330E-04
5.7444E-06	8.7982E-05	4.7262E 00	1.1077E-04	6.8416E 00	1.1583E-04
1.0980E-04	9.0514E-05	1.2707E 01	1.1330E-04	1.5569E 01	1.1836E-04
1.4864E-03	9.3046E-05	2.8647E 01	1.1583E-04	3.0970E 01	1.2090E-04
1.5785E-02	9.5578E-05	5.6922E 01	1.1836E-04	5.5433E 01	1.2343E-04
1.2922E-01	9.8109E-05	9.8959E 01	1.2090E-04	9.0186E 01	1.2596E-04
8.2709E-01	1.0064E-04	1.4962E 02	1.2343E-04	1.3310E 02	1.2849E-04
1.8111E 01	1.0570E-04	2.0116E 02	1.2596E-04	1.8139E 02	1.3102E-04
1.8577E 02	1.1077E-04	2.4323E 02	1.2849E-04	2.3175E 02	1.3356E-04
9.4659E 02	1.1583E-04	2.6763E 02	1.3102E-04	2.8068E 02	1.3609E-04
1.6632E 03	1.1836E-04	2.7443E 02	1.3356E-04	3.2583E 02	1.3862E-04
2.4659E 03	1.2090E-04	2.6709E 02	1.3609E-04	3.6635E 02	1.4115E-04
3.3773E 03	1.2596E-04	2.3221E 02	1.4115E-04	4.0211E 02	1.4368E-04
2.5242E 03	1.3102E-04	2.1421E 02	1.4368E-04	4.3343E 02	1.4621E-04
1.0906E 03	1.3609E-04	1.9873E 02	1.4621E-04	4.6107E 02	1.4875E-04
3.0952E 02	1.4115E-04	1.8634E 02	1.4875E-04	5.0858E 02	1.5381E-04
1.5835E 02	1.4368E-04	1.7045E 02	1.5381E-04	5.4887E 02	1.5887E-04
8.6296E 01	1.4621E-04	1.6248E 02	1.5887E-04	6.1852E 02	1.6900E-04
5.8807E 01	1.4875E-04	1.5980E 02	1.6394E-04	6.5066E 02	1.7407E-04
3.9261E 01	1.5381E-04	1.6382E 02	1.7407E-04	6.8168E 02	1.7913E-04
3.3962E 01	1.5887E-04	1.6831E 02	1.7913E-04	7.1187E 02	1.8419E-04
3.1197E 01	1.6394E-04	1.7363E 02	1.8419E-04	7.7320E 02	1.9432E-04
2.9325E 01	1.6900E-04	1.7950E 02	1.8926E-04	8.0652E 02	1.9938E-04
2.7919E 01	1.7407E-04	1.9355E 02	1.9938E-04	8.4252E 02	2.0445E-04
2.6748E 01	1.7913E-04	2.0179E 02	2.0445E-04	9.2258E 02	2.1457E-04
2.5650E 01	1.8419E-04	2.1071E 02	2.0951E-04	9.5792E 02	2.1964E-04
2.4579E 01	1.8926E-04	2.2792E 02	2.1964E-04	9.8391E 02	2.2470E-04
2.3481E 01	1.9432E-04	2.3286E 02	2.2470E-04	9.4337E 02	2.3483E-04
2.2388E 01	1.9938E-04	2.3327E 02	2.2977E-04	8.6251E 02	2.3989E-04
2.1196E 01	2.0445E-04	2.0325E 02	2.3989E-04	7.4256E 02	2.4496E-04
1.9861E 01	2.0951E-04	1.7408E 02	2.4496E-04	4.2467E 02	2.5508E-04
1.8276E 01	2.1457E-04	1.3849E 02	2.5002E-04	2.8283E 02	2.6015E-04
1.6514E 01	2.1964E-04	6.7513E 01	2.6015E-04	1.6738E 02	2.6521E-04
1.4542E 01	2.2470E-04	4.1400E 01	2.6521E-04	9.1460E 01	2.7028E-04
1.2440E 01	2.2977E-04	2.2419E 01	2.7028E-04	4.8064E 01	2.7534E-04
1.0235E 01	2.3483E-04	1.1400E 01	2.7534E-04	2.2137E 01	2.8040E-04
8.0373E 00	2.3989E-04	5.6734E 00	2.8040E-04	8.7352E 00	2.8547E-04
6.0264E 00	2.4496E-04	2.4514E 00	2.8547E-04	3.4336E 00	2.9053E-04
4.2035E 00	2.5002E-04	9.0677E-01	2.9053E-04	1.4133E 00	2.9559E-04
2.7844E 00	2.5508E-04	3.3874E-01	2.9559E-04	4.7559E-01	3.0066E-04
9.6703E-01	2.6521E-04	1.3553E-01	3.0066E-04	1.3472E-01	3.0572E-04
2.5567E-01	2.7534E-04	4.3796E-02	3.0572E-04	4.0557E-02	3.1079E-04
1.1428E-01	2.8040E-04	1.1914E-02	3.1079E-04	1.4437E-02	3.1585E-04
4.7190E-02	2.8547E-04	3.4433E-03	3.1585E-04	3.8459E-03	3.2091E-04
7.5055E-03	2.9559E-04	1.2156E-03	3.2091E-04	8.5302E-04	3.2598E-04
7.5793E-04	3.0572E-04	3.1628E-04	3.2598E-04	2.0294E-04	3.3104E-04
0.0000E 00	0.0000E 00	6.8481E-05	3.3104E-04	6.8441E-05	3.3610E-04
0.0000E 00	0.0000E 00	1.5647E-05	3.3610E-04	1.5484E-05	3.4117E-04
0.0000E 00	0.0000E 00	5.3236E-06	3.4117E-04	2.8844E-06	3.4623E-04
0.0000E 00	0.0000E 00	1.1907E-06	3.4623E-04	5.3702E-07	3.5129E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.6872E-07	3.5636E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	8.5177E-11	3.7155E-04

519163

0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	4.8472E-10	3.8168E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	2.8034E-11	3.9180E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.2732E-12	4.0193E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	5.2542E-14	4.1206E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	3.0509E-15	4.3231E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.4717E-16	4.4244E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	6.3041E-18	4.5257E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	3.1290E-19	4.7282E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.5767E-20	4.8295E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	6.9551E-22	4.9308E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	3.1745E-23	5.1333E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.6573E-24	5.2346E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	7.4927E-26	5.3359E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	3.2178E-27	5.5384E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.7373E-28	5.6397E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	8.0226E-30	5.7410E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	3.2679E-31	5.9435E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.8171E-32	6.0448E-04

SUMA= 5.8079E-02
SUMB= 2.7725E-02
SUMC= 9.1773E-02
TA= 1.2771E-04 TB= 1.7493E-04 TC= 1.9557E-04

519164


THEORETICAL CURVES - THE Y AXIS APPLIES TO ION SPECIES A
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0.27E 04
0.20E 04
0.14E 04
0.68E 03
0.00E 00
0.10E-03
0.12E-03
0.13E-03
0.15E-03
0.16E-03
0.18E-03
0.20E-03
0.21E-03
0.23E-03
0.24E-03
0.26E-03
0.27E-03
0.29E-0
3

519165

A	TIME	B	TIME	C	TIME
5.3337E-07	1.4368E-04	1.3343E-04	1.5381E-04	3.6475E-05	1.5381E-04
9.4340E-05	1.4875E-04	6.5640E-03	1.5887E-04	1.6442E-03	1.5887E-04
6.3127E-03	1.5381E-04	1.0647E-01	1.6394E-04	2.5838E-02	1.6394E-04
1.6656E-01	1.5887E-04	9.9407E-01	1.6900E-04	1.6360E 00	1.7407E-04
3.1251E 00	1.6394E-04	2.2774E 01	1.7913E-04	7.6566E 00	1.7913E-04
2.6843E 01	1.6900E-04	5.7249E 01	1.8419E-04	2.3578E 01	1.8419E-04
1.6446E 02	1.7407E-04	9.7683E 01	1.8926E-04	5.3304E 01	1.8926E-04
5.3821E 02	1.7913E-04	1.2333E 02	1.9432E-04	1.3884E 02	1.9938E-04
1.1251E 03	1.8419E-04	1.0951E 02	2.0445E-04	1.7661E 02	2.0445E-04
1.4402E 03	1.8926E-04	9.5273E 01	2.0951E-04	2.0649E 02	2.0951E-04
1.1249E 03	1.9432E-04	8.4936E 01	2.1457E-04	2.4866E 02	2.1964E-04
5.8452E 02	1.9938E-04	7.6709E 01	2.2470E-04	2.6603E 02	2.2470E-04
2.2336E 02	2.0445E-04	7.6529E 01	2.2977E-04	2.8287E 02	2.2977E-04
7.4382E 01	2.0951E-04	7.7944E 01	2.3483E-04	3.1872E 02	2.3989E-04
3.8734E 01	2.1457E-04	8.3871E 01	2.4496E-04	3.3711E 02	2.4496E-04
2.9229E 01	2.1964E-04	8.7565E 01	2.5002E-04	3.5563E 02	2.5002E-04
2.6628E 01	2.2470E-04	9.1518E 01	2.5508E-04	3.9317E 02	2.6015E-04
2.5352E 01	2.2977E-04	1.0006E 02	2.6521E-04	4.1234E 02	2.6521E-04
2.4713E 01	2.3483E-04	1.0459E 02	2.7028E-04	4.3191E 02	2.7028E-04
2.4371E 01	2.3989E-04	1.0929E 02	2.7534E-04	4.5220E 02	2.7534E-04
2.4208E 01	2.4496E-04	1.1933E 02	2.8547E-04	4.7337E 02	2.8040E-04
2.4137E 01	2.5002E-04	1.2459E 02	2.9053E-04	4.9516E 02	2.8547E-04
2.4109E 01	2.5508E-04	1.2997E 02	2.9559E-04	5.1754E 02	2.9053E-04
2.4116E 01	2.6015E-04	1.4103E 02	3.0572E-04	5.4056E 02	2.9559E-04
2.4106E 01	2.7028E-04	1.4670E 02	3.1079E-04	5.6412E 02	3.0066E-04
2.3861E 01	2.8040E-04	1.5251E 02	3.1585E-04	5.8791E 02	3.0572E-04
2.3320E 01	2.9053E-04	1.6517E 02	3.2598E-04	6.1205E 02	3.1079E-04
2.2461E 01	3.0066E-04	1.7200E 02	3.3104E-04	6.3680E 02	3.1585E-04
2.1884E 01	3.0572E-04	1.7882E 02	3.3610E-04	6.6326E 02	3.2091E-04
2.1242E 01	3.1079E-04	1.8940E 02	3.4623E-04	6.9126E 02	3.2598E-04
1.9619E 01	3.2091E-04	1.9008E 02	3.5129E-04	7.2050E 02	3.3104E-04
1.7530E 01	3.3104E-04	1.8625E 02	3.5636E-04	7.5053E 02	3.3610E-04
1.4903E 01	3.4117E-04	1.7681E 02	3.6142E-04	7.7751E 02	3.4117E-04
1.1731E 01	3.5129E-04	1.3199E 02	3.7155E-04	7.9633E 02	3.4623E-04
9.9823E 00	3.5636E-04	8.2869E 01	3.8168E-04	8.0254E 02	3.5129E-04
8.2421E 00	3.6142E-04	4.0593E 01	3.9180E-04	7.3705E 02	3.6142E-04
5.1367E 00	3.7155E-04	1.3577E 01	4.0193E-04	5.5795E 02	3.7155E-04
3.0290E 00	3.8168E-04	1.4269E 00	4.2219E-04	3.5167E 02	3.8168E-04
1.2835E 00	3.9180E-04	2.6972E-01	4.3231E-04	1.6214E 02	3.9180E-04
5.8652E-01	4.0193E-04	3.6944E-02	4.4244E-04	2.0103E 01	4.1206E-04
1.5212E-01	4.1206E-04	1.8947E-03	4.6270E-04	4.6398E 00	4.2219E-04
4.4258E-02	4.2219E-04	2.1554E-04	4.7282E-04	7.2819E-01	4.3231E-04
6.9690E-03	4.3231E-04	1.9527E-05	4.8295E-04	3.4161E-02	4.5257E-04
2.8022E-03	4.4244E-04	7.6696E-07	5.0321E-04	4.4338E-03	4.6270E-04
3.1761E-04	4.5257E-04	6.9182E-08	5.1333E-04	4.3194E-04	4.7282E-04
5.5605E-05	4.6270E-04	5.1501E-09	5.2346E-04	1.4515E-05	4.9308E-04
5.2587E-06	4.7282E-04	1.8013E-10	5.4372E-04	1.4799E-06	5.0321E-04
2.2256E-06	4.8295E-04	1.4451E-11	5.5384E-04	1.1659E-07	5.1333E-04
1.5895E-07	4.9308E-04	9.6807E-13	5.6397E-04	3.3790E-09	5.3359E-04
2.2469E-08	5.0321E-04	3.1811E-14	5.8423E-04	3.0989E-10	5.4372E-04
1.6462E-09	5.1333E-04	2.4138E-15	5.9435E-04	2.1956E-11	5.5384E-04
7.4401E-10	5.2346E-04	1.5257E-16	6.0448E-04	5.8150E-13	5.7410E-04
0.0000E 00	0.0000E 00	4.7972E-18	6.2474E-04	5.1089E-14	5.8423E-04
0.0000E 00	0.0000E 00	3.5454E-19	6.3486E-04	3.4205E-15	5.9435E-04
0.0000E 00	0.0000E 00	2.1655E-20	6.4499E-04	2.0067E-16	6.0448E-04
0.0000E 00	0.0000E 00	4.4340E-21	6.5512E-04	8.4367E-17	6.1461E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	7.3686E-18	6.2474E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	4.7880E-19	6.3486E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	2.7218E-20	6.4499E-04

0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	1.1008E-20	6.5512E-04
0.0000E 00	0.0000E 00	0.0000E 00	0.0000E 00	9.7908E-22	6.6524E-04

SUMA= 3.0290E-02
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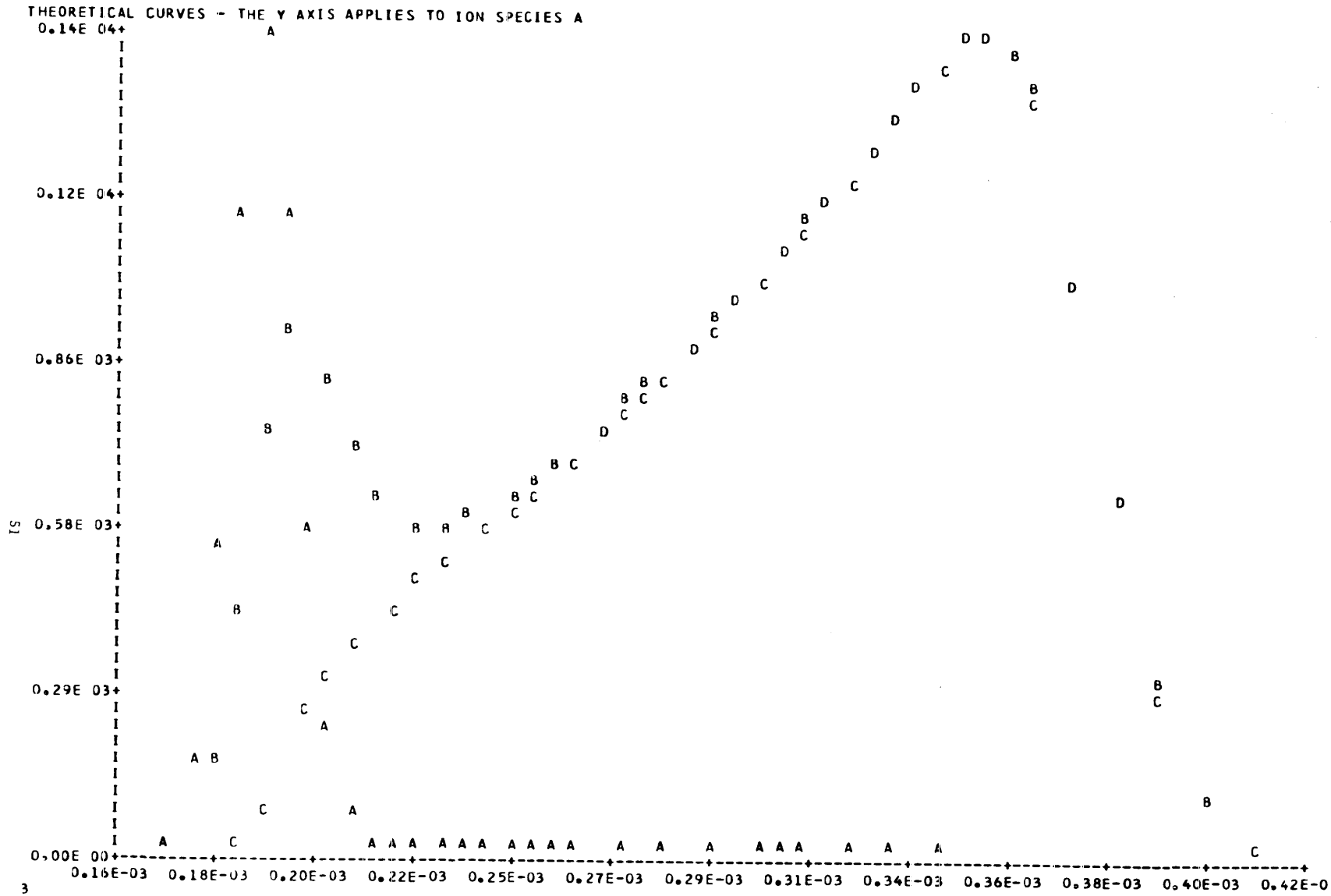
SUMC= 9.7792E-02
TA= 1.9666E-04 TB= 2.9478E-04 TC= 3.0584E-04

519167


THEORETICAL CURVES - THE Y AXIS APPLIES TO ION SPECIES A
0.14E 04
0.12E 04
0.86E 03
0.58E 03
0.29E 03
0.00E 00
SI
0.16E-03
0.18E-03
0.20E-03
0.22E-03
0.25E-03
0.27E-03
0.29E-03
0.31E-03
0.34E-03
0.36E-03
0.38E-03
0.40E-03
0.42E-0

519168

A	TIME	B	TIME	C	TIME
4.5954E-22	1.7407E-04	7.7327E-23	1.7407E-04	2.2191E-19	1.7913E-04
4.1456E-17	1.7913E-04	8.4423E-16	1.8419E-04	3.8334E-16	1.8419E-04
1.9250E-14	1.8419E-04	4.0778E-13	1.8926E-04	1.3350E-13	1.8926E-04
1.7574E-11	1.8926E-04	1.1660E-10	1.9432E-04	1.5690E-11	1.9432E-04
1.5097E-09	1.9432E-04	7.0647E-09	1.9938E-04	8.7171E-08	2.0445E-04
2.3672E-07	1.9938E-04	1.2168E-05	2.0951E-04	3.0917E-06	2.0951E-04
8.1500E-06	2.0445E-04	3.5104E-04	2.1457E-04	6.1846E-05	2.1457E-04
4.1711E-04	2.0951E-04	4.6064E-03	2.1964E-04	1.3159E-02	2.2470E-04
7.3709E-03	2.1457E-04	3.9752E-01	2.2977E-04	1.0750E-01	2.2977E-04
1.4920E-01	2.1964E-04	2.1707E 00	2.3483E-04	5.8690E-01	2.3483E-04
1.3845E 00	2.2470E-04	7.6175E 00	2.3989E-04	8.3243E 00	2.4496E-04
1.1479E 01	2.2977E-04	3.8000E 01	2.5002E-04	1.9856E 01	2.5002E-04
5.3827E 01	2.3483E-04	5.3164E 01	2.5508E-04	3.7239E 01	2.5508E-04
1.8559E 02	2.3989E-04	5.9679E 01	2.6015E-04	7.8534E 01	2.6521E-04
4.1131E 02	2.4496E-04	5.7034E 01	2.6521E-04	9.6000E 01	2.7028E-04
6.0617E 02	2.5002E-04	5.1040E 01	2.7028E-04	1.1033E 02	2.7534E-04
6.0802E 02	2.5508E-04	4.5669E 01	2.7534E-04	1.3230E 02	2.8547E-04
4.1600E 02	2.6015E-04	4.2095E 01	2.8040E-04	1.4151E 02	2.9053E-04
8.5318E 01	2.7028E-04	4.0306E 01	2.8547E-04	1.5017E 02	2.9559E-04
2.3320E 01	2.8040E-04	3.9819E 01	2.9053E-04	1.6708E 02	3.0572E-04
1.8180E 01	2.9053E-04	4.0154E 01	2.9559E-04	1.7553E 02	3.1079E-04
1.7526E 01	3.0066E-04	4.1052E 01	3.0066E-04	1.8400E 02	3.1585E-04
1.7550E 01	3.0572E-04	4.2352E 01	3.0572E-04	2.0100E 02	3.2598E-04
1.7689E 01	3.1079E-04	4.3939E 01	3.1079E-04	2.0949E 02	3.3104E-04
1.8148E 01	3.2091E-04	4.5684E 01	3.1585E-04	2.1809E 02	3.3610E-04
1.8731E 01	3.3104E-04	4.7533E 01	3.2091E-04	2.3683E 02	3.4623E-04
1.9313E 01	3.4117E-04	4.9445E 01	3.2598E-04	2.4769E 02	3.5129E-04
1.9834E 01	3.5129E-04	5.1409E 01	3.3104E-04	2.5958E 02	3.5636E-04
2.0069E 01	3.5636E-04	5.3437E 01	3.3610E-04	3.0198E 02	3.7155E-04
2.0267E 01	3.6142E-04	5.5564E 01	3.4117E-04	3.6531E 02	3.9180E-04
2.0549E 01	3.7155E-04	5.7842E 01	3.4623E-04	3.9981E 02	4.0193E-04
2.0693E 01	3.8168E-04	6.0451E 01	3.5129E-04	4.3606E 02	4.1206E-04
2.0647E 01	3.9180E-04	6.3316E 01	3.5636E-04	4.7403E 02	4.2219E-04
2.0425E 01	4.0193E-04	6.6604E 01	3.6142E-04	5.5696E 02	4.4244E-04
1.9943E 01	4.1206E-04	7.3381E 01	3.7155E-04	6.0086E 02	4.5257E-04
1.9264E 01	4.2219E-04	8.0638E 01	3.8168E-04	6.4308E 02	4.6270E-04
1.8412E 01	4.3231E-04	9.6447E 01	4.0193E-04	6.2265E 02	4.8295E-04
1.7375E 01	4.4244E-04	1.0501E 02	4.1206E-04	5.2276E 02	4.9308E-04
1.5859E 01	4.5257E-04	1.1394E 02	4.2219E-04	3.7138E 02	5.0321E-04
1.3911E 01	4.6270E-04	1.3327E 02	4.4244E-04	1.0510E 02	5.2346E-04
1.1487E 01	4.7282E-04	1.4357E 02	4.5257E-04	4.1173E 01	5.3359E-04
8.8074E 00	4.8295E-04	1.5275E 02	4.6270E-04	1.1911E 01	5.4372E-04
6.0785E 00	4.9308E-04	1.4763E 02	4.8295E-04	1.1424E 00	5.6397E-04
3.7322E 00	5.0321E-04	1.2248E 02	4.9308E-04	2.4060E-01	5.7410E-04
2.0093E 00	5.1333E-04	8.7636E 01	5.0321E-04	3.9287E-02	5.8423E-04
9.0235E-01	5.2346E-04	2.5214E 01	5.2346E-04	2.2438E-03	6.0448E-04
3.8816E-01	5.3359E-04	1.0659E 01	5.3359E-04	3.3615E-04	6.1461E-04
1.0918E-01	5.4372E-04	3.4280E 00	5.4372E-04	4.0223E-05	6.2474E-04
4.1753E-02	5.5384E-04	3.1864E-01	5.6397E-04	1.7449E-06	6.4499E-04
1.0271E-02	5.6397E-04	7.8127E-02	5.7410E-04	2.1526E-07	6.5512E-04
4.2122E-04	5.8423E-04	1.4379E-02	5.8423E-04	2.1384E-08	6.6524E-04
1.4727E-04	5.9435E-04	7.3326E-04	6.0448E-04	3.7645E-09	6.7537E-04
2.3593E-05	6.0448E-04	1.3126E-04	6.1461E-04	7.8248E-10	6.8550E-04
0.0000E 00	0.0000E 00	1.7567E-05	6.2474E-04	8.6162E-11	6.9563E-04
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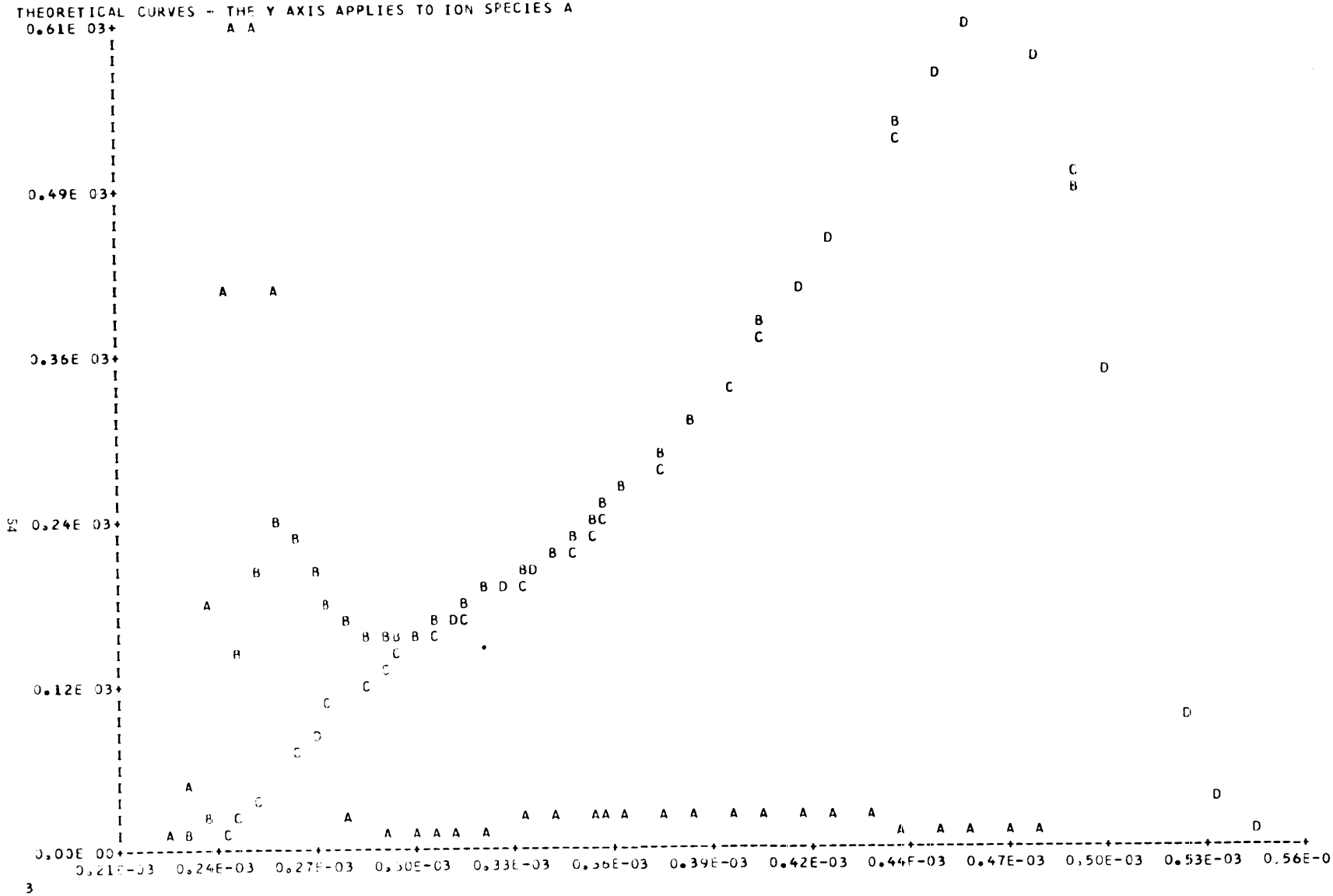
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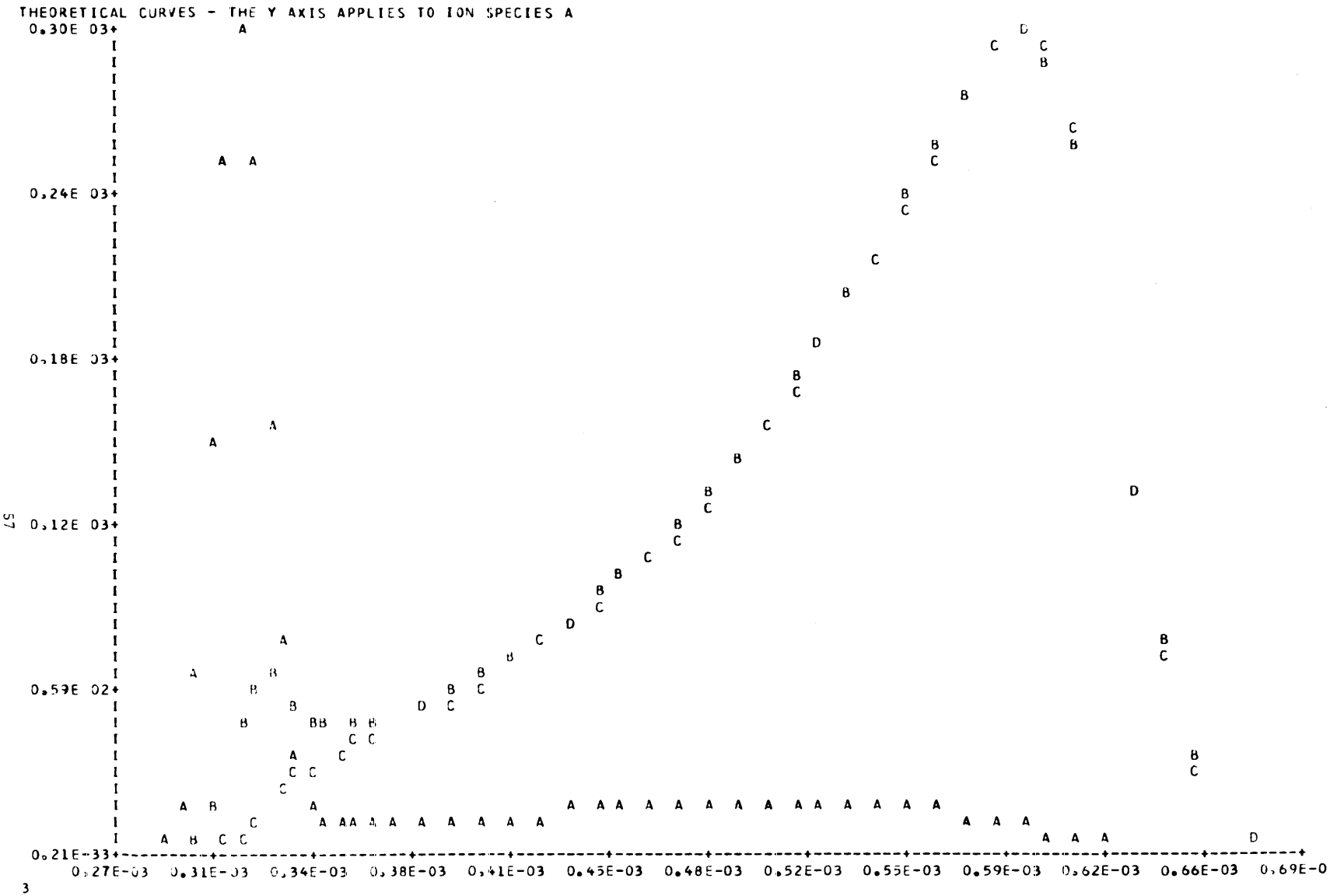
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DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author)	2a. REPORT SECURITY CLASSIFICATION
US Army Ballistic Research Laboratories Aberdeen Proving Ground, Maryland 21005	Unclassified
	2b. GROUP

3. REPORT TITLE

NUMERICAL MODEL FOR DRIFT TUBE ANALYSIS

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

5. AUTHOR(S) (First name, middle initial, last name)

G. E. Keller, M. R. Sullivan, L. M. Colonna-Romano, and M. D. Kregel

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
OCTOBER 1972	68	2

8a. CONTRACT OR GRANT NO.	9a. ORIGINATOR'S REPORT NUMBER(S)
b. PROJECT NO. RDT&E 1T061102B53A/15	REPORT NO. 1617
c.	9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)
d.	

10. DISTRIBUTION STATEMENT

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11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
	US Army Materiel Command Washington, DC 20315

13. ABSTRACT

A FORTRAN IV program has been written which uses an iterative technique to model ion transport and chemistry in a drift tube. The program, named MULTIGATE, uses finite difference calculus to generate time arrival histories at several points in the drift space for the case of three ion species undergoing populating and depopulating reactions and at the same time drifting with the electric field and diffusing in the radial and axial directions. To facilitate comparison with drift tube data, the computer output includes plots of the ionic currents versus time.

DD FORM 1 NOV 68 1473 REPLACES DD FORM 1473, 1 JAN 64, WHICH IS OBSOLETE FOR ARMY USE.

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14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Ionic Mobilities						
Diffusion Coefficients						
Ion-Molecule Reactions						
Drift Tubes						
Drift Tube Models						
Drift Tube Analysis						